

Annexure-II

W.E.F. 2017-18

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 preference will be given to candidates 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	FC	PMC.501	Computer Applications	2	1	-	2	10	15	15	10	50
	FC	PMC.502	Research Methodology & Biostatistics	2	1	-	2	10	15	15	10	50
3	CC	PMC.506	Modern Spectral and Chromatography Techniques	4	1	-	4	25	25	25	25	100
4	CC	PMC.507	Organic Chemistry-I	4	1	-	4	25	25	25	25	100
5	CC	PMC.508	Organic Synthesis -I (Practical)	-	-	4	2	-	-	-	-	50
6	CC	PMC.509	Spectral Analysis (Practical)	-	-	4	2	-	-	-	-	50
7	FC	PMC.597 - Seminar-I	Seminar	-	-	-	2	-	-	-	-	50
8	EC	XXX.###	Inter-Disciplinary Course (From Other Centres)	2	-	-	2	10	15	15	10	50
Opt any one course from following elective courses												
9	EC	PMC. 510	Logics of Organic Synthesis-I	4	1	-	4	25	25	25	25	100
		PMC. 511	Medicinal Chemistry									
		PMC. 512	Green Chemistry									
				18	5	8	24					600

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

A: Surprise Tests (Based on Objective Type Tests), and internal assessment including term paper and assignments.

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

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

SEMESTER 2

S. No	Type of Course	Paper Code	Course Title	L	T	P	Cr	% Weightage				E
								A	B	C	D	
1	CC	PMC.521	Organic Chemistry-II	4	1	-	4	25	25	25	25	100
2	CC	PMC.522	Organic Synthesis-II (Practical)	-	-	4	2	-	-	-	-	50
3	EC	PMC.523	Logics of Organic Synthesis-II	4	1	-	4	25	25	25	25	100
4	EC	PMC.524	Basics of Drug Design and Drug Action	4	1	-	4	25	25	25	25	100
5	CC	PMC.525	Computer Aided Drug Design (Practical)	-	-	4	2	-	-	-	-	50
6	FC	PMC.597-Seminar - II	Seminar	-	-	-	2	-	-	-	-	50
7	EC	XXX.###	Inter-Disciplinary Course (From Other Centres)	2	-	-	2	10	15	15	10	50
Opt any one course from following elective courses												
8	EC	PMC. 526	Chemistry of Natural Products	4	1	-	4	25	25	25	25	100
		PMC. 527	Advance Medicinal Chemistry									
		PMC. 528	Chromatographic Techniques									
				18	4	8	24					600

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

A: Surprise Tests (Based on Objective Type Tests), and internal assessment including term paper and assignments.

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

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

SEMESTER 3

S.No	Type of Course	Paper Code	Course Title	L	T	P	Cr	% Weightage				E
								A	B	C	D	
1	FC	PMC.597-Seminar-III	Seminar	-	-	-	2	-	-	-	-	50
2	CC	PMC.600	Thesis work and its mid-term evaluation (To be continued in semester 4)	-	-	-	22	-	-	-	-	-
							24					

FC: Foundation Course, **CC:** Core Course

A: Surprise Tests (Based on Objective Type Tests), and internal assessment including term paper and assignments.

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

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

SEMESTER 4

S.No	Type of Course	Paper Code	Course Title	L	T	P	Cr	% Weightage				E
								A	B	C	D	
1	CC	PMC.600	Thesis evaluation and viva-voce	-	-	-	24	-	-	-	-	-
							24					

CC: Core Course

A: Surprise Tests (Based on Objective Type Tests), and internal assessment including term paper and assignments.

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

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

Semester 1

Course Title: Computer Applications

Paper Code: PMC.501

L	T	P	Credits	Marks
2	1	0	2	50

Unit I **18 hours**

Fundamentals of Computers: Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean Algebra. Introduction to computer network and World Wide Web, Storage space, CPU and Memory. MS Word (Word Processing, Creating and Saving Documents, Text Formatting, Tables, Document Review Option, Inserting Table of Contents), Power point, Excel Sheet.

Unit II **18 hours**

Scientific information retrieval and web browsing: Introduction to various search engines such as Protein Data Bank, PubMed, NISCAIR, ACS, RSC, Elsevier, SciFinder, Google Scholar, Google patent, Espacenet, Beilstein databases, etc. Bibliography management and research paper formatting using reference software EndNote and reference manager. Sketching of molecules using ChemBio Draw, ChemSketch, etc.

Suggested Readings

1. Gookin, D. 2007. MS Word for Dummies. Wiley.
2. Harvey, G. 2007. MS Excel for Dummies. Wiley
3. Sinha, P.K. Computer Fundamentals. BPB Publications.
4. Bott, E. 2009. Windows 7 Inside Out. Microsoft Press.
5. Goel, A., Ray, S. K. 2012. Computers: Basics and Applications. Pearson Education India.

Course Title: Research Methodology & Biostatistics

Paper Code: PMC.502

L	T	P	Credits	Marks
2	1		2	50

Learning Outcomes:

Students who successfully complete this course will be able to:

- select and define an appropriate research problem and parameter
- Understand, design and set the objectives based on the literature search.
- Grasp the knowledge of protecting the research work through patent or copyright or trademarks.
- Type, cite and edit the references of their thesis/dissertation work
- Perform statistical calculations.

Unit 1

8 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

8 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.

Unit-3

20 hours

Biostatistics: Definition, application, sample size, importance of sample size, factors influencing sample size, dropouts, statistical tests of significance, type of significance tests, parametric tests (students “t” test, ANOVA, Correlation Coefficient, regression), nonparametric tests (Wilcoxon rank tests, analysis of variance, correlation, Chi square test), null hypothesis, P values, degree of freedom, interpretation of P values.

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.
8. Gookin, D. 2007. MS Word for Dummies. Wiley.
9. Harvey, G. 2007. MS Excel for Dummies. Wiley
10. Sinha, P.K. Computer Fundamentals. BPB Publications.
11. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
12. 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.
13. Bolton, S., & Bon, C. (2009). *Pharmaceutical statistics: practical and clinical applications*. CRC Press

Course Title: Modern Spectral & Chromatographic Techniques

Paper Code: PMC.506

L	T	P	Credits	Marks
4	1	-	4	100

Learning Outcomes

- Explain the general principle and theory of spectroscopy
- Describe the concept and instrumentation of UV-Vis, IR, NMR, Mass and Chromatographic techniques
- To study the spectra of the compounds and propose structure of the compounds
- Separation and identification of constituents of mixture by chromatographic techniques

Unit 1

14 hours

UV-Visible spectroscopy: Principle of UV-Visible Spectroscopy, Role of solvents, Chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rules, stereochemical aspects.

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

Unit 2

16 hours

Nuclear magnetic resonance spectroscopy: Magnetic properties of nuclei, Field and precession, Chemical shift concept, Isotopic nuclei, Reference standards and solvents. ^1H - NMR spectra, Relaxation processes, 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

14 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 enhancement (NOE), ^{13}C NMR spectra, their interpretation and application. DEPT techniques, Principle of 2-D NMR, Correlation spectroscopy (COSY) Homo COSY (^1H - ^1H COSY), Hetro COSY (^1H - ^{13}C COSY, HMQC), long range ^1H - ^{13}C COSY (HMBC), NOESY

Unit 4

16 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, MALDI and other recent advances in mass spectrometry

Chromatographic techniques: Principle and Classification of chromatography, Criteria for selection of stationary and mobile phase, Nature and types of mobile phases, Normal and reversed phase, Separation mechanism, Applications of Chromatography in different fields of Sciences, Column chromatography, TLC, LC, GC, HPTLC.

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. (Latest edition). *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 Dekker.
10. Silverstein, R. M., Webster, F. X., Kiemle, D., & Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley & Sons.
11. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.
12. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., New Delhi.
13. Sethi, P. D.; Sethi, R. (2007). *HPLC: High Performance Of Liquid Chromatography*, Vol 2, CBS
14. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental Methods of Analysis*, CBS Publishers and Distributors.

Course Title: Organic Chemistry-I

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PMC.507

Learning Outcomes:

Students who successfully complete this course will be able to:

- Understand the stereochemistry, spatial arrangement of atoms/groups and apply it on the course of reactions and mechanism prediction.
- The basics of organic chemistry will enable understand students to build knowledge in drug synthesis and their interaction with receptors

Unit 1

22 hours

Stereochemistry: IUPAC nomenclature of organic molecules, Elements of symmetry, Chirality, Projection formulae [Flywedge, 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, D/L, R/S, E/Z and *cis/trans* 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, .

Unit 2

18 hours

Aliphatic nucleophilic substitution reaction: The S_N^2 , S_N^1 , mixed S_N^2 and S_N^1 and SET mechanism, The S_N^i 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 S_N^2 and S_N^1 mechanisms.

Aromatic nucleophilic substitution: The S_N^{Ar} , bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

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, Vilsmeier–Haack reaction.

Unit 3**16 hours**

Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, 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, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

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. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry* Organic Chemistry Oxford press, 2nd edition
2. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
3. Mc Murry J., *Organic Chemistry*, Asian Book Pvt. Ltd, 8th edition, New Delhi
4. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
5. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, New Delhi-110002.
6. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
7. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
8. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., 3rd edition, New Delhi.
9. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
10. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, New York.
11. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
12. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., 3rd edition, New Delhi.

13. Robert and Casereo, (1977). *Basic principle of Organic Chemistry*, Addison-Wesley, 2nd edition.
14. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10th edition.
15. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition.
16. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

Course Title: Organic Synthesis-I (Practical)

L	T	P	Credits	Marks
-	-	4	2	50

Paper Code: PMC.508

1. Demonstration of Stereochemical aspects of the compounds through molecular models.
2. Awareness to various glasswares and plasticwares used in the organic synthesis.
3. Awareness to handling, storage and disposal of hazardous chemicals and their MSDS.
4. Thin layer chromatography: 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
5. Purification of a given organic compound through crystallization, fractional distillation or column chromatography.
6. **Organic Synthesis:** Single or multi- steps synthesis of organic compounds. Aspects such as conversion, yield, selectivity, effluent treatment, atom economy, etc. should be paid attention. TLC should be used to monitor the reaction. (attempt any five)
 - a) Synthesis of an anticancer stilbene via Wittig reaction
 - b) Synthesis of chalcones via Claisen-Schmidt condensation.
 - c) Preparation of vanillyl alcohol from vanillin
 - d) Reduction of 3-nitroacetophone using $\text{NaBH}_4/\text{LiAlH}_4$
 - 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.

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. (latest edition). *Text book of practical organic chemistry*, Pearson
6. Williamson, K.L., Heath, 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 Title: Spectral Analysis (Practical)

L	T	P	Credits	Marks
-	-	4	2	50

Paper Code: PMC. 509

- 1) Exercises of structure elucidation of unknown compounds *via* spectral interpretation of ^1H , ^{13}C NMR, IR, UV and Mass.
- 2) Hands on experience with various analytical instruments such as FT-IR, UV-vis spectrophotometer, GC-MS, and HPLC.

Suggested Readings:

1. Adams,R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan 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. (latest edition). *Text book of practical organic chemistry*, Pearson
6. Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D.Cand 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

Elective Courses

Course Title: Logics of Organic Synthesis-I

L	T	P	Credits	Marks
4	1	-	4	100

Paper Code: PMC.510

Learning outcome: Students who successfully complete this course will be able to

- Propose and determine the mechanism and feasibility of a chemical reaction
- Apply principle of photochemistry in various chemical transformations
- Explore various metal and non-metal reagents towards oxidation and reduction reactions
- Name different fused and bridged heterocyclic compounds and perform their synthesis through different methods

Unit 1 16 hours

Reaction mechanism, structure and reactivity: Types of mechanisms, types of reactions, 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, Di π – methane rearrangement. Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction Singlet molecular oxygen reactions

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-Ponndorf-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, imidazole, pyrazole, 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 heteroatom: Synthesis and reactions of pyrylium salts and pyrones, coumarins, chromones, pyridine, pyrimidine *etc.*

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 International (P) Ltd., 5th edition, New Delhi.
5. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (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). *Heterocyclic 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., (2014). *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 Chemistry* Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, 5th edition, New York.
19. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7th edition, India.
20. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
21. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
22. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
23. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
24. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3rd edition, UK.
25. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.

Course Title: Medicinal Chemistry

L	T	P	Credits	Marks
4	1	-	4	100

Paper Code: PMC.511

Learning Outcomes:

Students who successfully complete this course will be able to:

- Understand basics concepts of drugs, their effects and screening.
- Know how drugs interact with various types of enzymes and receptors
- Know the process of drug discovery and its progress.

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: Green Chemistry

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PMC.512

Learning outcome:

Students who successfully complete this course will be able to

- Understand various aspects of green chemistry for sustainable development
- Utilize ionic liquids and solid supported reaction conditions to reduce or eliminate use of volatile organic solvents
- Use water as solvent in chemical transformations
- Utilize MW and sonicator in organic synthesis

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-alkylation, S-alkylation. Darzens reaction, Williamsons synthesis, Wittig reaction, Click Chemistry. 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. Ahluwalia, 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.
4. Matlack, A. (2010). Introduction to green chemistry. CRC Press.
5. Ahluwalia, V. K. (2011). Green Chemistry: Greener Alternatives to Synthetic Organic Transformations. Alpha Science International.

Course Title: Seminar

Paper Code: PMC.597-Seminar-I

L	T	P	Credits	Marks
-	-	4	2	50

Semester 2

Course Title: Organic Chemistry-II

Paper Code: PMC.521

L	T	P	Credits	Marks
4	1	0	4	100

Learning Outcomes:

Students who successfully complete this course will be able to:

- Understand the disconnection approaches apply it on synthetic strategies and mechanism prediction.
- understand the basics of photochemical reactions that will enable understand students to build knowledge in drug synthesis

Unit 1

14 hours

Reactive intermediates: Generation, structure and reactions of carbocation, carbanion, free radicals, carbenes, nitrenes, benzyne, 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, regioselectivity, 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-Benzilic 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 Asymmetric Epoxidation, Ene, Barton, Hofmann-Löffler Fretag, Shapiro reaction, Chichibabin Reaction.

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 $[l]$ 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* 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 International (P) Ltd., 5th edition, New Delhi.
6. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age International (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). *Heterocyclic 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 Chemistry* 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 Synthron 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 Title: Organic Synthesis-II (Practical)

L	T	P	Credits	Marks
-	-	4	2	50

Paper Code: PMC.522

1. Separation and purification of organic compounds by column chromatography: Separation of mixture of *ortho* and *para* mixture and cis/trans mixture. The column chromatography should be monitored by TLC.
2. **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 allylic alcohols via Baylis-Hillman reaction using DABCO as a catalyst under neat condition and their characterization through various spectroscopic techniques.
 - h) Preparation of homoallyl alcohols via Barbier type reaction under aqueous condition using Indium as a catalyst.
 - i) Suzuki reaction of 3,4-dimethoxy phenyl boronic acid with aryl halides using Pd(PPh₃)₄ as a catalyst.
3. Exercises on identification of compounds *via* combined spectral interpretation of ¹H, ¹³C NMR, IR, UV and Mass along with 2-D NMR spectra.

Suggested Readings:

1. Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan 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. (Latest edition). *Text book of practical organic chemistry*, Pearson
6. Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D.C. and Co., Lexington, MA.

Course Title: Logics of Organic Synthesis-II

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PMC.523**Learning Outcomes:**

Students who successfully complete this course will be able to:

- Understand the asymmetric synthesis, chiral resolution and apply it on the resolution of chiral drugs.
- The basics of organic chemistry will enable understand students to build knowledge in drug synthesis and their interaction with receptors

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, Wittig, 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 Organoboranes viz hydroboration with BH₃-THF, dicyclohexyl borane, disiamyl borane, teryl borane, 9-BBN and disopinacamphyl borane, 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, Baker's yeast, D. D. Q, Lead tetraacetate, Prevost Hydroxylation, Wilkinson's catalyst, Phase transfer catalysts: Quaternary ammonium and Phosphonium salts, Crown ethers, Merfield 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., Wothers, 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 Vol. IV* Wiley-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 Jürgen, 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. Davies 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 Title: Basics of Drug Design and Drug Actions

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PMC.524**Learning outcome:** Students who successfully complete this course will be able to

- Apply the knowledge of drug-receptor interactions for understanding drug mechanism
- Utilize the knowledge of ligand interactions with the active site of receptor in novel drug design and discovery
- Apply the knowledge on QSAR for novel drug designing

Unit 1**14 hours**

Interactions of enzyme/receptor with 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 oxamiquine, salbutamol, cimitidine and captopril. Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, barbiturates, and taxol analogs. Principles of prodrug design, Serendipitous discovery of leads e.g. Penicillin and Librium.

In silico methods: Introduction to Quantitative Structure Activity Relationship (QSAR) studies. 2-D QSAR, QSAR parameters. 3-D QSAR, CoMFA and CoMSIA. Molecular docking, Pharmacophore mapping and virtual screening.

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 Williams & Wilkins.

Course Title: Computer Aided Drug Design (Practical)

L	T	P	Credits	Marks
-	-	4	2	50

Paper Code: PMC.525

Following practicals utilizing the available softwares such as ChemBio Draw, Autodock, Schrodinger, etc. need to be conducted.

- 1) Determination of LogP, MR, HBD and HBA of selected drugs
- 2) Calculation of ADMET properties of drugs molecules and their analysis
- 3) Homology Modelling based experiments.
- 4) Practical based on 2D and 3D-QSAR of drug molecules.
- 5) Docking and virtual screening based experiments.

Course Title: Seminar

L	T	P	Credits	Marks
-	-	4	2	50

Paper Code: PMC.597 - Seminar -II

Elective Courses

Course Title: Chemistry of Natural Products

Paper Code: PMC.526

L	T	P	Credits	Marks
4	1	0	4	100

Learning Outcomes

- Students will become familiar with various types of natural products
- Students will understand the role of natural products in living organisms, their biosynthesis and will have a greater understanding of organic synthesis
- To understand the role of natural products in drug discovery and development

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 Verlag.
8. Thomson, R.H. (2008). *The Chemistry of Natural Products*, Springer, 1st edition.

Course Title: Advance Medicinal Chemistry

Paper Code: PMC.527

L	T	P	Credits	Marks
4	1	0	4	100

Learning Outcomes

- Students will become familiar with various types of drugs
- Students will be able to design new drugs as antiviral, antidepressant and cardiovascular agents

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, Didanosine, Nevirapine, Delaviridine, 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, antiarrhythmics, 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. Nogard, 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. 528

L	T	P	Credits	Marks
4	1	0	4	100

Learning outcomes

- Students will be familiar with comprehensive knowledge of the theoretical principles of chromatographic methods on molecular level
- To understand basic principles in managing chromatographic equipment and evaluation of its efficiency
- To analyse different samples (products of organic synthesis, environmental and food samples) using gas and high performance liquid chromatography
- To select optimal method for the sample preparation and analysis as well as to carry out data processing and result analysis

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. Heftmann, E. (2004). *Chromatography*, Vol 69 A, Elsevier
2. Lundanes, E.; Reubsæet, L.; Greibrakk, T. (2013). *Chromatography: Basic Principles, Sample preparations and related methods*, Wiley.
3. Sethi, P. D.; Sethi, R. (2007). *HPLC: High performance of liquid chromatography*, Vol 2, CBS
4. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.

5. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors.

Semester 3

Course Title: Seminar
Paper Code: PMC.597-Seminar - III

L	T	P	Credits	Marks
-	-	4	2	50

Course Title: Thesis work and its mid-term evaluation (to be continued in semester 4)

Paper Code: PMC.600

L	T	P	Credits
-	-	-	22

Semester 4

PMC.600

Thesis work & Evaluation

L	T	P	Credits
-	-	-	24