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

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	PPL.501	Computer Applications	2	1	-	2	10	15	15	10	50
2	FC	PPP.502	Computer Applications - Practical	-	-	4	2	-	-	-	-	50
3	FC	PPL.503	Research Methodology	2	1	-	2	10	15	15	10	50
4	FC	PPL.504	Biostatistics	2	1	-	2	10	15	15	10	50
5	EC	PPL.505	Organic Chemistry-I	4	1	-	4	25	25	25	25	100
6	CC	PPL.506	Advances in Pharmacognosy and Phytochemistry	4	1	-	4	25	25	25	25	100
7	CC	PPP.507	Pharmacognosy, Phytochemistry and spectral analysis - Practical	-	-	4	2	-	-	-	-	50
8	FC	PPS.598	Seminar	-	-	-	2	-	-	-	-	50
9	EC	XXX. ###	Inter-Disciplinary Course (From Other Centres)	2	-	-	2	10	15	15	10	50
Opt any one course from following elective courses												
10	EC	PPL. 508	Spectral Analysis and Chromatographic Techniques	4	1	-	4	25	25	25	25	100
		PPL. 509	Medicinal Chemistry									
		PPL. 510	Logics of Organic Synthesis									
				20	**6**	**8**	**26**					**650**

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

A: Surprise Tests (minimum three): Based on Objective Type Tests

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	EC	PPL.511	Organic Chemistry -II	4	1	-	4	25	25	25	25	100
2	CC	PPL.512	Phytochemical techniques and analysis	4	1	-	4	25	25	25	25	100
3	CC	PPP.513	Extraction and isolation of natural products - Practical	-	-	4	2	-	-	-	-	50
4	EC	PPL.514	Basics of drug design and drug action	4	1	-	4	25	25	25	25	100
5	CC	PPP.515	Molecular modeling of natural products - Practical	-	-	4	2	-	-	-	-	50
6	FC	PPS.599	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	PPL. 516	Chemistry of Natural Products	4	1	-	4	25	25	25	25	100
		PPL. 517	Advance Medicinal Chemistry									
		PPL. 518	Green Chemistry									
				18	**4**	**8**	**24**					**600**

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

A: Surprise Tests (minimum three): Based on Objective Type Tests
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	PPS. 699	Seminar	-	-	-	2	-	-	-	-	50
2	CC	PPT.600	Thesis work and its mid-term evaluation (To be continued in semester IV)	-	-	-	22	-	-	-	-	550
							24					**600**

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

A: Surprise Tests (minimum three): Based on Objective Type Tests

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	PPT.600	Thesis evaluation and viva-voce	-	-	-	24	-	-	-	-	600
							24					**600**

CC: Core Course

A: Surprise Tests (minimum three): Based on Objective Type Tests
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: PPL.501

L	T	P	Credits	Marks
2	0	0	2	50

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

- Use and search various search engines for literature survey their research work.
- Type, cite and edit the references of their thesis/dissertation work

Unit I **9 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.

Unit II **9 hours**

MS-Word: Introduction to Word Processing, Creating and Saving Documents, Text Formatting, Tables, Document Review Option, Mail Merge, Inserting Table of Contents, Reference Management.

Unit III **9 hours**

Applications Software: Introduction to MS Paint, Notepad, Spreadsheet applications, Presentation applications, Internet browsers and Image processing applications.

Unit IV **9 hours**

World Wide Web: Origin and concepts, Latency and bandwidth, searching the internet, Advanced web-search using Boolean logic, Networking fundamentals.

Text books:

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.

Suggested Readings:

1. Bott, E. 2009. Windows 7 Inside Out. Microsoft Press.
2. Goel, A., Ray, S. K. 2012. Computers: Basics and Applications. Pearson Education India.

Course Title: Computer Applications-Practical
Paper Code: PPP.502

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 Web Browsers
3. Optimizing web search: Google advanced search, Boolean operators, Literature search using Google Scholar, HighWire, Pubmed, Scifinder, etc.
4. Bibliography management and research paper formatting using reference software EndNote
5. Creating a functional website using HTML

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 Title: Research Methodology

Paper Code: PPL.503

L	T	P	Credits	Marks
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.

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 Title: Biostatistics

Paper Code: PPL.504

L	T	P	Credits	Marks
2	-	-	-	50

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

- Understand basic descriptive and inferential statistics including the concepts and principles of research design and statistical inference.
- Perform and interpret descriptive and inferential statistical techniques including the construction of tables and graphs, t-tests, Chi-square tests, and regression analysis.
- Communicate with statisticians and other professionals about the planning, implementation, and interpretation of analytic studies.
- Use appropriate software packages to solve analytical problems.

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 Title: Organic Chemistry-I

Paper Code: PPL.505

L	T	P	Credits	Marks
4	1	0	4	100

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_N2, S_N1, mixed S_N2 and S_N1 and SET mechanism, The S_Ni 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_N2 and S_N1 mechanisms.

Aromatic nucleophilic substitution: The S_NAr, 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 Inrternational (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: Advances in Pharmacognosy and Phytochemistry

Paper Code: PPL.503

L	T	P	Credits	Marks
4	1	0	4	100

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

- Understand and learn the natural products based drug discovery and pharamcognostical and cultivation methods of medicinal plants

Unit 1 **12 hours**

Natural Products as drugs: Historical background, present status and future scope of natural products in drug discovery; Lipinski rule; Different approaches to drug discovery- Rational (sense), irrational (non-sense) and antisense approach; Selection of natural sources for drug development based on random, phytoconstituents and ethnopharmacological records

Unit 2 **14 hours**

Biotechnological aspects: DNA recombinant technology, mutation, polyploidy and hybridization to improve the quality of vegetable drugs and their constituents, chemical races. Plant growth regulators and their use, scope and limitations in Pharmacognosy, Effect of growth hormones on production of secondary plant metabolites, Pharming in plants, Transgenic medicinal plants *Catharanthus roseus*, *Papaver somniferum*, *Panax ginseng*.

Unit 3 **20 hours**

Pharmacognostic aspects of tissue culture: Plant tissue culture techniques & its application in relation to phytopharmaceuticals: Techniques of initiation & maintenance of various types of cultures, Immobilized cell techniques (survey of recent advances), Germ plasm storage, biotransformation studies, recent advances in elicitor techniques and production of biological active constituents in static, suspension, multiple shoot cultures. Bioreactors for production of biologically active constituents and other applications of plant tissue culture techniques. Biosynthetic potential of tissue cultures and factors affecting production of secondary metabolites by tissue culture techniques. *Azadirachta indica, Melia azadirachta, Cassia fistula*

Unit 4 **14 hours**

Cultivation methods developed in India for the following medicinal plants and commercial significance: *Stevia rebaudiana, Podophyllum hexandrum, Ocimum sanctum, Colchium officinalis, Curcuma longa, Taxus baccata, Glycyrrhiza glabra, Azadirachta indica.*

Unit 5 **12 hours**

Discovery of Lead Molecules from Natural Sources and their Contribution to Modern Therapeutics: Vinca alkaloids, podophyllum lignans, quinine, artemisinin, digitalis glycosides, paclitaxel, Volatile oils and aromatherapy, Industrial scenario of nutraceuticals in India

Suggested Readings

1. W.C. Evans, Trease and Evans, Pharmacognosy, 15th edition, W.B. Sounders & Co., London, 2002.
2. Tyler, V.E., Brady, L.R. and Robbers, J.E., Pharmacognosy, 9th Edn., Lea and Febiger, Philadelphia, 1988.
2. H.E. Street, Plant Tissue and Cell Culture, Blackwell Scientific Publication, London, 1977.
3. A.N. Kalia, Textbook of Industrial Pharmacognosy, CBS Publishers, New Delhi
4. Margaret L, Vickery and Brian Vickery, Secondary Plant Metabolism, The Macmillan Press Ltd, London, 1981.
5. R Endress, Plant cell Biotechnology, Springer-Verlag, Berlin, 1994.
6. Torseel KBG. Natural Product Chemistry. John Wiley and Sons, New York. Latest Edition.
7. Harborne JB. Phytochemical Methods. Chapman and Hall, London. Latest Edition.
8. Atal, C.K., Kapur, B.M., Cultivation and Utilization of Medicinal and Aromatic Plants, R.R.L., Jammu.
9. Staba, E.J., Applied and Fundamental Aspects of Plant Cell, Tissue and organ (Reivert J. and Y.P.S., Bajaj Ed.), Berlin.
10. Tabata, M., Plant Tissue Culture and its Biotechnological Applications, Berlin.
11. Reinhard, E., Tissue Culture and Plant Science, Academic Press, London.
12. Gene Cloning and DNA Analysis,-An Introduction (2001) Brown T. A., Blackwell Publishing
13. Principles of Gene Manipulation and Genomics (2001) - Primrose S. B. & Twyman R. M, Blackwell Publishing
14. Hopkins, W.G. and Huner, N.P.A. (2010). *Introduction to Plant Physiology*. 4th Edition, John Wiley and Sons, Inc.
15. Taiz, L. and Zeiger, E. (2010). *Plant Physiology*. Sinauer Associates Inc. U.S.A.
16. Ali, M. (2011). Pharmacognosy (Pharmacognosy and Phytochemistry). CBS Publisher & Distributors P Ltd.
17. Kokate, CK, Purohit, AP and Gokhale, SB. (2011). Pharmacognosy. Nirali Prakashan.
18. Denston, TC. (2012). A Textbook of Pharmacognosy. Kellock Robertson Press.
19. Mukherjee, PK. (2012). Quality Control of Herbal Drugs, Business Horizons; Reprint 2012 edition.
20. Rogers, K. (2012). Out of Nature: Why Drugs from Plants Matter to the Future of Humanity, University of Arizona Press; 1 edition.
21. Kar, A. (2007). Pharmacognosy and Pharmaco- biotechnology, New Age International Pvt Ltd Publishers.

Course Title: Pharmacognosy, Phytochemistry and Spectral Analysis-Practical

Paper Code: PPP.507

L	T	P	Credits	Marks
-	-	4	2	50

Microscopical methods of examining crude drugs, Determination of stomatal index, Palisado ration, Determination of stomatal number, Determination of total ash, Determination of acid insoluble, water soluble and sulphated ash, Determination of Iodine value, Method of alkaloid determination

Maceration, Hot continuous extraction, percolation, Ultrasound-assisted, Microwave-assisted, Accelerator-assisted solvent extraction, spraying reagents for identification of different secondary metabolites: terpenoids, Flavonoids, alkaloids, steroids, carbohydrates

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.

1. Study of molecules using molecular models
2. Exercises of structure elucidation of unknown compounds *via* spectral interpretation of ^{1}H, ^{13}C NMR, IR, UV and Mass.
3. Hands on experience with various analytical instruments such as FT-IR, UV-vis spectrophotomer, GC-MS, microwave synthesizer, solvent extractor and HPLC.

Suggested Readings:

1. Handa, S.S, Khanuja, SPS, Longo, G and D.D.Rakesh. Extraction technologies for Medicinal and Aromatic plants. International Centre for Science and High technology, CRC Press, USA
2. Protocol for testing Ayurvedic, Siddha, and Unani Medicines, Department of Ayush, Government of India
3. Khandelwal, KR. (2008). Practical Pharmacognosy, Nirali Prakashan; 18th edition.
4. Zafar, R and Gandhi, N. (2007). Practical Pharmacognosy, CBS Publishers & Distributors.

Course Title: Seminar
Paper Code: PPS.598

L	T	P	Credits	Marks
-	-	4	2	50

Elective Courses

Course Title: Spectral Analysis and Chromatographic Techniques

Paper Code: PPL. 508

L	T	P	Credits	Marks
4	1	0	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. ^{1}H- 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 **16 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 (^{1}H-^{1}H COSY), Hetro COSY (^{1}H-^{13}C COSY, HMQC), long range ^{1}H-^{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

Unit 5 **12 hours**

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 dnd Their Applications***,** Marcel Deckker.
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: Medicinal Chemistry

Paper Code: PPL.509

L	T	P	Credits	Marks
4	1	-	4	100

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

- Understand basics concepts of drugs, their effects and screening.
- Know how does drug 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: Logics of Organic Synthesis

Paper Code: PPL.510

L	T	P	Credits	Marks
4	1	-	4	100

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, lead tetraacetate, 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, 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 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., (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). *Heterocyc1ic 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 Chemistr*y Elsevier, 3rd edition, UK.
25. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.

Semester 2

Course Title: Organic Chemistry-II

Paper Code: PPL.511

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, 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 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 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 Title: Phytochemical techniques and analysis

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PPL.512

Learning Outcomes:

Students who successfully complete this course will be able to:

- Understand the extraction techniques, isolation of plant derived products
- learn standardization of the plant based drugs.

Unit 1 **18 hours**

Extraction techniques: Different extraction methods (maceration, percolation, hot continuous extraction, hydro distillation) including advanced extraction techniques like supercritical fluid extraction, accelerated solvent extraction, microwave-assisted extraction, ultrasound assisted extraction, solid-phase micro extraction including headspace techniques;

Unit 2 **18 hours**

Isolation techniques: Fractionation and solvent partitioning, General principles, classification, normal and reversed phase, bonded phase, separation mechanisms, Chromatographic separations including column chromatography, vacuum liquid chromatography, flash chromatography, prep TLC, Droplet counter-current chromatography (DCCC), ion exchange chromatography, centrifugal counter-current chromatography (CCC), Centrifugally accelerated chromatography, HPLC, HPTLC, GC

Unit 3 **18 hours**

Structural characterization: Purification techniques for isolated phytochemicals, Chemical assays for different natural products, introduction to different techniques of characterization of bioactive constituents such as flavonoids, terpenoids, alkaloids and steroids

Unit 4 **18 hours**

Plant Drug Standardization: Macroscopic: Organoleptic methods including morphology, sampling, preliminary examination and foreign matter; Microscopic: General microscopy, Histochemistry, Quantitative microscopic**;** Physico-chemical: Solubility, specific gravity, optical rotation, refractive index, melting point, swelling index, foaming index, moisture content, ash value, extractive values including volatile oil; General methods of assays for alkaloids, steroids, terpenoids, flavonoids, glycosides, tannins and coumarins. Fingerprint profiling of crude drugs and single and multicomponent herbal preparation, stability testing of natural products

Suggested Readings

1. Sethi, P. D.; Sethi, R. (2007). *HPLC: High performance of liquid chromatography*, Vol 2, CBS Publishers and Distributors.
2. Silverstein, R.M. (2006). *Spectrometric Identifications of Organic Compound***s**, John Wiley, 6th edition, .
3. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, 7th edition, New York.
4. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors, 2nd edition.

5. S.S.Handa, S.P.S.Khanuja, G.Longo, D.D.Rakesh. Extraction technologies for Medicinal and Aromatic plants. International Centre for Science and High technology, CRC Press, USA

Course Title: Extraction and Isolation of Natural Products - Practical

Paper Code: PPP.513

L	T	P	Credits	Marks
-	-	4	2	50

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.

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 Title: Basics of Drug Design and Drug Actions

Paper Code: PPL.514

L	T	P	Credits	Marks
4	1	0	4	100

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 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 Title: Molecular Modelling of Natural Products-Practical

Paper Code: PPP.515

L	T	P	Credits	Marks
-	-	4	2	50

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.

Course Title: Seminar

Paper Code: PPP.599

L	T	P	Credits	Marks
-	-	4	2	50

Elective Courses

Course Title: Chemistry of Natural Products

Paper Code: PPL.516

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, 3nd 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 Title: Advance Medicinal Chemistry

Paper Code: PPL.517

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, 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 Title: Green Chemistry

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PPL.518

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 soild 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-alkylalion, 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. 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 Title: Seminar

Paper Code: PPS.699

L	T	P	Credits	Marks
-	-	4	2	50

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

Paper Code: PPT.600

L	T	P	Credits	Marks
-	-	-	22	550

Semester 4

Course Title: Thesis Evaluation and Viva Voce

Paper Code: PPT.600

L	T	P	Credits	Marks
-	-	-	24	600