

ANNEXURE -VI

W.E.F. 2018-19

Department of 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	PPP.501	Computer Applications	2	1	-	2	10	15	15	10	50
2	FC	PPP.502	Research Methodology	2	1	-	2	10	15	15	10	50
	FC	PPP. 503	Biostatistics	2	1	-	2	10	15	15	10	50
3.	CC	PPP. 506	Pharmacognosy	4	1	-	4	25	25	25	25	100
4.	CC	PPP. 507	Modern Spectral and Chromatography Techniques	4	1	-	4	25	25	25	25	100
5.	CC	PPP 508	Pharmacognosy & Phytochemistry (Practical)			4	2	-	-	-	-	50
6.	CC	PPP.509	Spectral Analysis (Practical)	-	-	4	2	-	-	-	-	50
7.	FC	PPP. 597 (Seminar-1)	Seminar	-	-	-	2	-	-	-	-	50
8.	EC	XXX. ###	Inter-Disciplinary Course (From Other Centres)	2	1	-	2	10	15	15	10	50
Opt any one course from following elective courses												
9	EC	PPP 510	Organic Chemistry-1	4	1	-	4	25	25	25	25	100
		PPP. 511	Medicinal Chemistry									
		PPP. 512	Logics of Organic Synthesis									
				20	7	8	26					650

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 TestC: Mid-Semester Test – II: Based on Subjective Type TestD: 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	PPP.521	Herbal and Cosmetic Analysis	4	1	-	4	25	25	25	25	100
2	CC	PPP. 522	Phytochemical techniques and analysis	4	1	-	4	25	25	25	25	100
3	CC	PPP 523	Chemistry of Natural Products	4	1	-	4	25	25	25	25	100
4	CC	PPP.524	Extraction and isolation of natural products (Practical)	-	-	4	2	-	-	-	-	50
5	CC	PPP.525	Computer Aided Drug Design (Practical)	-	-	4	2	-	-	-	-	50
6	FC	PPP. 597 (Seminar-II)	Seminar	-	-	-	2	-	-	-	-	50
7.	EC	XXX. ###	Inter-Disciplinary Course (From Other Centres)	2	1	-	2	10	15	15	10	50
Opt any one course from following elective courses												
8	EC	PPP 526	Basics of Drug Design and Drug Action	4	1	-	4	25	25	25	25	100
		PPP 527	Organic Chemistry-II									
		PPP. 528	Advance Medicinal 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 3

S. No	Type of Course	Paper Code	Course Title	L	T	P	Cr	% Weightage				E
								A	B	C	D	
Opt any one course from following elective courses												
1	EC	PPP. 551	Regulatory Toxicology	4	1	-	4	25	25	25	25	100
2		PPP. 528	Advance Medicinal Chemistry									
3		PPP. 552	Green Chemistry									
4	CC	PPP.600	Thesis work and its mid-term evaluation (To be continued in semester 4)	-	-	-	20	-	-	-	-	-
				4	1	-	24					100

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	PPP.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

L	T	P	Credits
2	1	-	2

Paper Code: PPP.501

Learning Outcomes:

Upon successful completion of this course, the student will be able to:

- Use different operating system and their tools easily.
- Use word processing software, presentation software, spreadsheet software and latex.
- Understand networking and internet concepts.
- Use computers in every field like teaching, industry and research.

Unit 1 9 hours

Computer Fundamentals: Introduction to Computer, Input devices, Output Devices, Memory (Primary and Secondary), Concept of Hardware and Software, C.P.U., System bus, Motherboard, Ports and Interfaces, Expansion Cards, Ribbon Cables, Memory Chips, Processors, Software: Types of Software, Operating System, User Interface of popular Operating System, Introduction to programming language, Types of Computer.

Unit 2 9 hours

Computer Network: Introduction to Computer Network, Types of Network: LAN, WAN and MAN, Topologies of Network, Internet concept, WWW.

Word Processing using MS Word: Text creation and Manipulation; Table handling; Spell check, Hyper-linking, Creating Table of Contents and table of figures, Creating and tracking comments, language setting and thesaurus, Header and Footer, Mail Merge, Different views, Creating equations, Page setting, Printing, Shortcut keys.

Unit 3 9 hours

Presentation Tool: Creating Presentations, Presentation views, Working on Slide Transition, Making Notes Pages and Handouts, Drawing and Working with Objects, Using Animations, Running and Controlling a Slide Show, Printing Presentations, Shortcut keys.

Spread Sheet: Entering and editing data in cell, Basic formulas and functions, deleting or inserting cells, deleting or inserting rows and columns, printing of Spread Sheet, Shortcut keys.

Unit 4 9 hours

Use of Computers in Education and Research: Data analysis tools, e-Library, Search engines related to research such as Protein Data Bank, PubMed, NISCAIR, ACS, RSC, Elsevier, SciFinder, Google Scholar, Google patent, Espacenet, Beilstein databases etc., Research paper editing tools like Latex. Bibliography management and research paper formatting using reference software EndNote and reference manager. Sketching of molecules using ChemBio Draw, ChemSketch etc.

Suggested Readings:

1. Sinha, P.K. Computer Fundamentals. BPB Publications.
2. Goel, A., Ray, S. K. 2012. Computers: Basics and Applications. Pearson Education India.
3. Microsoft Office Professional 2013 Step by Step
<https://ptgmedia.pearsoncmg.com/images/9780735669413/samplepages/9780735669413.pdf>
4. Gookin, D. 2007. MS Word for Dummies. Wiley.
5. Harvey, G. 2007. MS Excel for Dummies. Wiley
6. Bott, E. 2009. Windows 7 Inside Out. Microsoft Press.
7. Goel, A., Ray, S. K. 2012. Computers: Basics and Applications. Pearson Education India.

Course Title: Research Methodology

Paper Code: PPP.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.

Unit 1

18 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

18 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.
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.

Course Title: Biostatistics

Paper Code: PPP.503

L	T	P	Credits	Marks
2	1		2	50

Learning Objectives:

To provide the understanding and use of Statistical techniques for students of other departments.

Unit 1

9 hours

Descriptive Statistics: Meaning, need and importance of statistics. Attributes and variables. Measurement and measurement scales. Collection and tabulation of data. Diagrammatic representation of frequency distribution: histogram, frequency polygon, frequency curve, ogives, stem and leaf plot, pie chart.

Unit II

9 hours

Measures: Measures of central tendency, dispersion (including box and whisker plot), skewness and kurtosis. Linear regression and correlation (Karl Pearson's and Spearman's) and residual plots.

Unit III

9 hours

Random variables and Distributions: Discrete and continuous random variables. Discrete Probability distributions like Binomial, Poisson and continuous distributions like Normal, F and student-t distribution.

Unit IV

9 hours

Differences between parametric and non-parametric statistics. Confidence interval, Errors, Levels of significance, Hypothesis testing.

Parametric tests: Test for parameters of Normal population (one sample and two sample problems) z-test, student's t-test, F and chi-square test and Analysis of Variance (ANOVA).

Non-Parametric tests: One sample: Sign test, signed rank test, Kolmogrov-Smirnov test, run test. Critical difference (CD), Least Significant Difference (LSD), Kruskal-Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks.

Recommended Books:

1. P. L. Meyer, *Introductory Probability and Statistical Applications*, Oxford & IBH Pub, 1975.
2. R. V. Hogg, J. Mckean and A. Craig, *Introduction to Mathematical Statistics*, Macmillan Pub. Co. Inc., 1978.

Suggested Readings:

1. F. E. Croxton and D. J. Cowden, *Applied General Statistics*, 1975.
2. P. G. Hoel. *Introduction to Mathematical Statistics*, 1997.
3. G. Norman, and D. Streiner. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
4. 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.
5. S. Bolton and C. Bon (2009). *Pharmaceutical statistics: practical and clinical applications*. CRC Press

Course Title: Pharmacognosy

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PPP.506

Learning Outcomes

- Know advancements in cultivation and production of drugs
- Know the process like genetic engineering in medicinal plants for higher yield of Phytopharmaceuticals
- To know various aspects of plant drug standardization
- Use the biotechnological techniques for obtaining and improving the quality of natural products/medicinal plants

Unit 1 **16 hours**

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

Unit 2 **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 3 **16 hours**

Plant Drug Standardization: Macroscopic: Organoleptic methods including morphology, sampling, preliminary examination and foreign matter; Microscopic: General microscopy, Histochemistry, Quantitative microscopic; Determination of stomatal index, Palisade ratio, Physico-chemical: Solubility, specific gravity, optical rotation, refractive index, melting point, swelling index, foaming index, moisture content, ash value, iodine value, extractive values including volatile oil, Method of alkaloid determination

Unit 4 **20 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*.

Suggested Readings

1. W.C. Evans, Trease and Evans, Pharmacognosy, 15th edition, W.B. Saunders & 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: Modern Spectral and Chromatography Techniques

Paper Code: PPP. 507

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. 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. ¹⁹F, ¹⁵N, ³¹P

Unit 3

14 hours

Principles of FT-NMR with reference to ¹³C NMR, Free induction decay, Average time domain and frequency domain signals, Spin-spin and spin-lattice relaxation phenomenon, Nuclear Overhauser enhancement (NOE), ¹³C NMR spectra, their interpretation and application. DEPT techniques, Principle of 2-D NMR, Correlation spectroscopy (COSY) Homo COSY (¹H-¹H COSY), Hetro COSY (¹H-¹³C COSY, HMQC), long range ¹H-¹³C 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: Pharmacognosy & Phytochemistry (Practical)

L	T	P	Credits	Marks
-	-	4	2	50

Paper Code: PPP.508

Microscopical methods of examining crude drugs, Determination of stomatal index, Palisade ratio, 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

Detection of phytoconstituents by TLC methods, spraying reagents for identification of different secondary metabolites such as Alkaloids, Steroids, Triterpenoids and their glycosides and saponins, Anthracene glycosides, Flavanoids and their glycosides Coumarins, Tannins

Suggested Readings:

1. Khandelwal, K.R. (2008). Practical Pharmacognosy, Pragati Books Pvt. Ltd
2. Virensah (2010). Text Book of Pharmacognosy and Phytochemistry, Elsevier
3. Clarke, H.T. (1975). *A Handbook of Organic. Analysis Qualitative and Quantitative.* Edward Arnold Publishers Ltd London.

Course Title: Spectral Analysis (Practical)

L	T	P	Credits	Marks
-	-	4	2	50

Paper Code: PPP 509

Learning Outcomes:

Students who successfully complete this course will be able to:

List of experiments

1. Interpretation of spectra and structure determination by UV, IR, NMR and Mass Spectroscopy of the following compounds

Morphine, ephedrine, paclitaxel, flavonoids, terpenoids, steroids, carbohydrates

Course Title: Seminar

Paper Code: PPP.597 (Seminar-I)

L	T	P	Credits	Marks
-	-	-	2	50

Elective Courses

Course Title: Organic Chemistry - 1

Paper Code: PPP.510

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_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: Medicinal Chemistry

L	T	P	Credits	Marks
4	1	-	4	100

Paper Code: PPP.511

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

L	T	P	Credits	Marks
4	1	-	4	100

Paper Code: PPP.512

Learning outcomes: 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-Ponndorf-Verley reduction, Dissolving metal reductions, metal hydride reductions using NaBH₄, LiAlH₄, 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.

Semester 2

Course Title: Herbal and Cosmetic Analysis

Paper Code: PPP.521

L	T	P	Credits	Marks
4	1	0	4	100

Learning outcomes:

- Determination of herbal remedies and regulations
- Analysis of natural products and monographs
- Determination of Herbal drug-drug interaction
- Principles of performance evaluation of cosmetic products

Unit 1 14 hours

Herbal remedies- Toxicity and Regulations: Herbals vs Conventional drugs, Efficacy of herbal medicine products, Validation of Herbal Therapies, Pharmacodynamic and Pharmacokinetic issues. Herbal drug standardization: WHO and AYUSH guidelines.

Unit 2 14 hours

Adulteration and Deterioration: Introduction, types of adulteration/substitution of herbal drugs, Causes and Measure of adulteration, Sampling Procedures, Determination of Foreign Matter, DNA Finger printing techniques in identification of drugs of natural origin, heavy metals, pesticide residues, phototoxin and microbial contamination in herbal formulations. Regulatory requirements for setting herbal drug industry: Global marketing management, Indian and international patent law as applicable herbal drugs and natural products and its protocol.

Unit 3 14 hours

Testing of natural products and drugs: Effect of herbal medicine on clinical laboratory testing, Adulterant Screening using modern analytical instruments, Regulation and dispensing of herbal drugs, Stability testing of natural products, protocol. Monographs of Herbal drugs: Study of monographs of herbal drugs and comparative study in IP, USP, Ayurvedic Pharmacopoeia, American herbal Pharmacopoeia, British herbal Pharmacopoeia, Siddha and Unani Pharmacopoeia, WHO guidelines in quality assessment of herbal drugs.

Unit 4 14 hours

Herbal drug-drug interaction: WHO and AYUSH guidelines for safety monitoring of natural medicine, Spontaneous reporting schemes for bio drug adverse reactions, bio drug-drug and bio drug-food interactions with suitable examples. Challenges in monitoring the safety of herbal medicines.

Unit 5 16 hours

Evaluation of cosmetic products: Determination of acid value, ester value, saponification value, iodine value, peroxide value, rancidity, moisture, ash, volatile matter, heavy metals, fineness of powder, density, viscosity of cosmetic raw materials and finished products. Study of quality of raw materials and general methods of analysis of raw material used in cosmetic manufacture as per BIS. Indian Standard specification laid down for sampling and testing of various cosmetics in finished forms such as baby care products, skin care products, dental products, personal hygiene preparations, lips sticks. Hair products and skin creams by the Bureau Indian Standards.

Suggested Readings

1. Pharmacognosy by Trease and Evans
2. Pharmacognosy by Kokate, Purohit and Gokhale
3. Quality Control Methods for Medicinal Plant, WHO, Geneva
4. Pharmacognosy & Pharmacobiotechnology by Ashutosh Kar
5. Essential of Pharmacognosy by Dr.S.H.Ansari
6. Cosmetics – Formulation, Manufacturing and Quality Control, P.P. Sharma, 4th edition, Vandana Publications Pvt. Ltd., Delhi
7. Indian Standard specification, for raw materials, BIS, New Delhi.
8. Indian Standard specification for 28 finished cosmetics BIS, New Delhi
9. Harry's Cosmeticology 8th edition
10. Suppliers catalogue on specialized cosmetic excipients
11. Wilkinson, Moore, seventh edition, George Godwin. Poucher's Perfumes, Cosmetics and Soaps
12. Hilda Butler, 10th Edition, Kluwer Academic Publishers. Handbook of Cosmetic Science and Technology, 3rd Edition,
13. A.N. Kalia, Textbook of Industrial Pharmacognosy, CBS Publishers, New Delhi
14. Gene Cloning and DNA Analysis,-An Introduction (2001) Brown T. A., Blackwell Publishing
15. Mukherjee, PK. (2012). Quality Control of Herbal Drugs, Business Horizons; Reprint 2012 edition.

Course Title: Phytochemical techniques and analysis

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PPP.522**Learning Outcomes:**

Students who successfully complete this course will be able to:

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

Unit 1**20 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**20 hours**

Isolation techniques: Fractionation and solvent partitioning, Chromatographic separations including column chromatography, vacuum liquid chromatography, flash chromatography, prep TLC, Droplet counter-current chromatography (DCCC), ion exchange chromatography, Membrane filtration based upon size, size exclusion/gel chromatography, semi and preparative HPLC, centrifugal counter-current chromatography (CCC), Centrifugally accelerated chromatography,

Unit 3**12 hours**

Fingerprint profiling of crude drugs and single and multicomponent herbal preparation, stability testing of natural products, HPLC, HPTLC, and GC.

Unit 4**20 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

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 Compounds*, 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
6. Sarker, S. D., & Nahar, L. (2012). An introduction to natural products isolation. Natural products isolation, 1-25.

7. Bhutani, K.K., Singh, I.P., Jachak S. M.,(2017). Analytical Profiles of selected medicinal plants. ISBN (10): 93-85046-07-1.

Course Title: Chemistry of Natural Products

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PPP.523**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: Forskolin, Rohitukine (Flavopiridol).

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, Marker degradation.

Unit 4 **9 hours**

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

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, oligosaccharides, polysaccharides.

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: Extraction and Isolation of Natural Products (Practical)

Paper Code: PPP.524

L	T	P	Credits	Marks
-	-	4	2	50

Maceration, Hot continuous extraction, percolation, Ultrasound-assisted, Microwave-assisted, Accelerator-assisted solvent extraction, record the percentage yield and physical status of the respective extracts for phytochemical screening.

- a) Isolation of caffeine from tea leaves.
- b) Isolation of Piperanine from *Piper ornatum*.
- 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 lycopene from tomatoes.
- f) Isolation of β -carotene from carrots.
- g) FT-IR, UV-vis spectrophotometer, GC-MS, solvent extractor and HPLC of natural products

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.
3. Khandelwal, K.R. (2008). *Practical Pharmacognosy*, Pragati Books Pvt. Ltd
4. Virensah (2010). *Text Book of Pharmacognosy and Phytochemistry*, Elsevier

Course Title: Computer Aided Drug Design (Practical)

Paper Code: PPP.525

L	T	P	Credits	Marks
-	-	4	2	50

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

Paper Code: PPP.597 (Seminar-II)

L	T	P	Credits	Marks
-	-	4	2	50

Elective Course

Course Title: Basics of Drug Design and Drug Action

Paper Code: PPP.526

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 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 stereo chemical 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, Stereo chemical 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, 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.

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 Williams & Wikins.

Course Title: Organic Chemistry-II**Paper Code: PPP.527**

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:** Synthons, 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 Assymmetric Epoxidation, Ene, Barton, Hofmann-Löffler 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 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 $[l,j]$ shifts; Cope and Claisen rearrangements; Explanation for the mechanism of sigmatropic reactions by (i) symmetry properties of HOMO (ii) 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 International (P) Ltd., 5th edition, New Delhi.
6. Bansal, R.K. (2010). *Heterocyclic 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: Advance Medicinal Chemistry

L	T	P	Credits	Marks
4	1	0	4	100

Paper Code: PPP.528

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*, Royal 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.

SEMESTER 3 Course Title: Regulatory Toxicology**Paper Code: PPP. 551**

L	T	P	Cr	Marks
4	1	0	4	100

Unit I Introduction to Toxicology 18 hours

Pharmacoeology introduction and concepts, General Nature of Pharmaceutical Toxicants in Environment, concepts & their effects; Basic Probit analysis; Toxicants – Toxicity, mechanism of toxicity - Acute, sub-acute, chronic, dose effect, LD50, LC50 and response safe limits; IT, IC, LD₈₀, LD₉₀, LCIC, Dose response relationship, concentration response relationship; Influence of route of administration; determination of toxicity of pharmaceutical wastes.

Unit II Toxic Mechanisms 18 hours

Bioaccumulation and Biomagnification of pharmaceutical wastes materials in food chain, detoxification, bioconcentration; Toxicology of major pharmaceutical wastes, their biotransformation, biomonitoring, residual effects; bioindicator– definition, groups and examples.

Unit III Bioassays 18 hours

Concepts, types, characteristics and significance of bioassay; Bioassay test models and classification - Microbial, algal, invertebrates and alternative toxicity tests; Immunotoxicity, histotoxicity, cell toxicity with respect to pharmaceutical effluents. Toxicity of pharmaceutical wastes – Legislative perspectives.

Unit IV Regulatory Requirements in Pharmaceutical Industries and Allied Area 18 hours

ICH, European FDA, USFDA guidelines for Acute toxicity, Chronic toxicity testing, Reproductive toxicology, Genotoxicity (carcinogen and teratogen) Occupational hazards in Pharmaceutical industries, Safety requirements and Measures; Occupationally induced illness, non-occupational illness, discomfort at work, Occupational diseases, Occupational cancer, Occupational dermatitis; Radiation, fire and explosion hazards Hazards; occupational health practice; risk assessment techniques for accidental release of toxic and inflammable materials; Role of WHO in occupational health related to pharmaceutical wastes. Occupational health Standards - ISO. NCE, NME, Biosimilar. Botanical, Herbal and Ayurvedic dietary supplements.

Suggested readings:

1. Tatiya, Ratan raj (2013) Elements of industrial hazards: Health, safety, environment and loss prevention Taylor and Francis
2. Theodore, Louis (2012) Environmental health and hazard risk assessment : Principles and calculations, CRC Press
3. Wong, Ming H. (Ed.) (2013) Environmental contamination: Health risks and ecological restoration, CRC press
4. Manahan, Stanley E. (2013) Fundamentals of environmental and toxicological chemistry: Sustainable sciences, CRC press

5. Jjemba, P. K. (2008). Pharma-ecology: the occurrence and fate of pharmaceuticals and personal care products in the environment. John Wiley & Sons.

Course Title: Advance Medicinal Chemistry

Paper Code: PPP.528

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, Delavirdine, 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:

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

18. 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
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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.

SEMESTER 4

S.No	Type of Course	Paper Code	Course Title	L	T	P	Cr	% Weightage				E
								A	B	C	D	

1	CC	PPP.600	Thesis evaluation and viva-voce	-	-	-	24	-	-	-	-	600
							24					600

CC: Core Course

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

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

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

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

J: Total Marks

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