Centre for Chemical and Pharmaceutical Sciences 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 also having valid GPAT score.

SEMESTER 1

			EMIES) I 121\								
							9,	6 We	ightag	ge		
S.No	Paper	Course Title	L	T	P	Cr					E	
5.110	Code	Course Title	L	1	1	CI	A	В	C	D	E	
		Computer Applications										
1	PPP.501	1 11	2	1	-	2	10	15	15	10	50	
		Organic Chemistry-I										
2	PPP.502		4	1	-	4	25	25	25	25	100	
		Advances in										
		Pharmacognosy and										
3	PPP.503	Phytochemistry	4	1	-	4	25	25	25	25	100	
		Laboratory of										
	DDD 504	Pharmacognosy and										
4	PPP.504	Phytochemistry	-	-	4	2	-	-	-	-	50	
_	DDD 505	Spectral Analyses-			,						50	
5	PPP.505	Practical	-	-	4	2	-	-	-	-	50	
	DDD 506	Computer Applications			1	2					50	
6	PPP.506	-Practical	-	-	4	2	-	-	-	-	50	
7	PPP. 507	Seminar	-	-	4	2	-	-	-	-	50	
		Inter-Disciplinary										
		Course (From Other										
8	XXX.###	Departments)	2	-	-	2	10	15	15	10	50	
Ont any	one course	from following elective	course	S								
opt uny	PPP. 508	Spectral Analyses	course									
	PPP. 509	Medicinal Chemistry										
9	111.507	Logics of Organic	4	1	-	4	25	25	25	25	100	
	PPP. 510	Synthesis										
	FFF. 310	Synthesis	16	4	16	24					600	
Interdisc	oinlinery co	urses offered by Chemical					ulty (E	or etu	donts	of othe		
Centres)	-	urses offered by Cheffical	anu i	11411114	iceuiic	ai rac	uity (1	or stu	uents	or onic	1	
01		Diseases and Medicines	2			2	10	15	15	10	50	
01	111.331	Chemicals of Everyday		_		4	10	13	13	10	50	
02	PPP.552	Life	2	_	_	2	10	15	15	10	50	
02	111.332	Spectroscopy in Drug		_			10	13	13	10	50	
		Development and										
03	PPP.553	Analyses	2	_	_	2	10	15	15	10	50	
03	111.333	Tilalyses		-	-		10	13	13	10	50	
L					<u> </u>	<u> </u>	1					

A: Continuous Assessment: Based on Objective Type Tests

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

L: Lectures T: Tutorial P: Practical Cr: Credits SEMESTER 2

S.No	Paper	Course Title	L	Т	P	Cr	9,	6 We	ighta	ge	E
2.110	Code	Course Tine	L	1	ľ	_ Cr	A	В	С	D	E
1	PPP.511	Organic Chemistry-II	4	1	-	4	25	25	25	25	100
2	PPP.512	Phytochemical techniques and analysis	4	1	_	4	25	25	25	25	100
3	PPP.513	Basics of Drug Design and Dug Actions	4	1	-	4	25	25	25	25	100
4	PPP.514	Extraction and Isolation of Natural Products- Practical	-	-	4	2	_	1	-	1	50
5	PPP.515	Analyses and Molecular Modeling of Natural		-	4	2	_	1	-	1	50
6	PPP.516	Seminar	-	_	4	2	_	_	_	_	50
7	XXX.###	Inter-Disciplinary Course (From Other Departments)	2	_	_	2	10	15	15	10	50
Opt any	one course	from following elective	course	S							
8	PPP. 517	Chemistry of Natural Products Advance Medicinal	4	1	-	4	25	25	25	25	100
	PPP. 518 PPP. 519	Chemistry Green Chemistry									
			16	4	12	24					600
Interdise Centres	Interdisciplinary courses offered by Chemical and Pharmaceutical Faculty (For students of other								er		
01	PPP.551	Diseases and Medicines	2	-	-	2	10	15	15	10	50
02	PPP.552	Chemicals of Everyday Life	2	-	_	2	10	15	15	10	50
03	PPP.553	Spectroscopy in Drug Development and		-	-	2	10	15	15	10	50

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

L: Lectures T: Tutorial P: Practical Cr: Credits SEMESTER 3

C No	Paper	Course Title	т	T	ъ	C	9,	6 We	ighta	ge	\mathbf{E}
S.No	Code	Course Title	\mathbf{L}	T	P	Cr	A	В	C	D	L
1	PPP. 601	Research Methodology	2	1	1	2	10	15	15	10	50
2	PPP. 602	Biostatistics	2	ı	ı	2	10	15	15	10	50
3	PPP. 603	Biostatistics - Practical	-	-	4	2	_	-	-	-	50
4	PPP. 604	Mid-Term Evaluation of Thesis	-	-	4	18					450
			04	-	4	24					600

SEMESTER 4

S.No	Paper	Course Title	L	Т	P	Cr	9,	6 We	ighta	ge	E
5.110	Code	Course Title	L	1	r	Cr	A	В	C	D	L
1	PPP. 605	Medicinal Chemistry of Anticancer Agents	4	1	ı	4	25	25	25	25	100
2	PPP. 606	Thesis Evaluation and Viva Voce	-	-	-	20	-	-	-	-	500
			04	-	4	24					600

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

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

Semester 1

Course Tile: Computer Applications

Paper Code: PPP.501

L	T	P	Credits	Marks
2	0	0	2	50

Unit 1 18 hours

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

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

Unit 2 18 hours

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

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

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

Course Tile: Organic Chemistry-I

Paper Code: PPP.502

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 22 hours

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

Unit 2 18 hours

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

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

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

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

Unit 3 16 hours

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

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, Regio- and

chemoselectivity, orientation and reactivity, hydroboration, alkylation, epoxidation and hydroxylation, addition of halogen polar reagents to alkenes.

Unit 4 16 hours

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

- 1. Finar, I.L., (2003). Organic Chemistry Vol. 1. Pearson Education, 4th edition.
- 2. Mc Murry J., Organic Chemistry, Asian Book Pvt. Ltd, 8th edition, New Delhi
- 3. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
- 4. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, New Delhi-110002.
- 5. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age Insternational (P) Ltd., 5th edition, New Delhi.
- 6. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
- 7. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., 3rd edition, New Delhi.
- 8. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
- 9. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, New York.
- 10. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
- 11. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., 3rd edition, New Delhi.
- 12. Robert and Casereo, (1977). *Basic principle of Organic Chemistry*, Addison-Wesley, 2nd edition.
- 13. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10th edition.
- 14. Sykes, P., (1997). A Guide Book to Mechanism in Organic Chemistry, Prentice Hall, 6th edition.
- 15. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

Course Tile: Advances in Pharmacognosy and Phytochemistry

Paper Code: PPP.503

L	T	P	Credits	Marks
4	1	0	4	100

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 Tile: Laboratory of Pharmacognosy and Phytochemistry-Practical

Paper Code: PPP.504

L	Т	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.

Study of molecules using molecular models

Suggested Readings:

- 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 Tile: Spectral Analysis-Practical

Paper Code: PPP.505

]	Ĺ	T	P	Credits	Marks
-	-	-	4	2	50

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

Course Tile: Computer Applications-Practical

Paper Code: PPP.506

L	T	P	Credits	Marks
-	ı	4	2	50

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

Suggested Readings:

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

Course Tile: Seminar Paper Code: PPP.507

L	T	P	Credits	Marks
	-	4	2	50

Elective Courses

Course Tile: Spectral Analyses

Paper Code: PPP.508

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 18 hours

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

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

Unit 2

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

Unit 3 18 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 enhanced (NOE), ¹³C NMR spectra, their interpretation and application. APT and 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, DEPT and 2D INADEQUATE experiments and their application, Solid-state NMR.

Unit 4 18 hours

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

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

- 5. Khopkar, S.M. (2007). *Basic Concepts of Analytical Chemistry*, New Age International Pvt Ltd.
- 6. Melinda J.D., (2010). Introduction to solid NMR Spectroscopy, Wiley India Pvt Ltd
- 7. Mendham, J.; Denney, R.C.; Barnes, J. D.; Thomas, M. J. K. (2003). *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Pvt. Ltd., New Delhi.
- 8. Pavia, D.L.; Lampman, G. M. (2010). *Introduction to Spectroscopy*, G. S. Kriz, Harcourt College, NY.
- 9. Popov, A.I.; Halenga, K. (1991). *Modern NMR techniques and their Applications*, Marcel Deckker.
- 10. Silverstein, R.M. (2006). Spectrometric Identifications of Organic Compounds, John Wiley.
- 11. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.
- 12. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors.
- 13. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., New Delhi.

Course Tile: Medicinal Chemistry

Paper Code: PPP.509

L	T	P	Credits	Marks
4	1	-	4	100

Unit 1 10 hours

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

Unit 2 20 hours

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

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

Unit 3 22 hours

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

Unit 4 20 hours

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

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

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

Course Tile: Logics of Organic Synthesis

Paper Code: PPP.510

L	T	P	Credits	Marks
4	1	ı	4	100

Unit 1 16 hours

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

Unit 2 16 hours

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

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

Unit 3 18 hours

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

Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Pondorff-Verley reduction, Dissolving metal reductions, metal hydride reductions using 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, oxazoles and thiazoles.
- (c) Benzo-fused five-membered and six membered heterocycles: Synthesis and reactions of indoles, benzofurans and benzimidazoles, benzothiazoles.

- (d) Six-membered heterocycles with one heteroatom: Synthesis and reactions of pyrylium salts and pyrones, coumarins, chromones.
- (e) Six-membered heterocycles with 2 or more nitrogen atoms: Synthesis, reactivity, aromatic character and importance of the following heterocycles: 1,2,3-triazoles, 1,2,4-triazoles, tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine and tetrazines.

- 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 Insternational (P) Ltd., 5th edition, New Delhi.
- 5. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Insternational (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., (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.

Interdisciplinary Courses

Course Tile: Diseases and Medicines

Paper Code: PPP.551

L	T	P	Credits	Marks
2	0	0	2	50

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

Unit 1 18 hours

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

Unit 2 18 hours

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

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

Course Tile: Chemicals of Everyday Life

Paper Code: PPP.552

L	T	P	Credits	Marks
2	0	0	2	50

Unit 1 9 hours

Chemicals and safety

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

Unit 2 9 hours

Common chemical processes

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

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

Unit 3 9 hours

Chemistry of small bioactive molecules

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

Abused substances like morphine, Cannabis, Cocaine etc.

Unit 4 9 hours

Green chemical processes

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

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

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

Course Title: Spectroscopy in Drug Development and Analyses

Paper Code: PPP.553

S	L	T	P	Credits	Marks
	2	-	0	2	50

Unit 1 9 hours

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

Unit 2 hours

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

Unit 3 hours

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

Unit 4 hours

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

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

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

Semester 2

Course Tile: Organic Chemistry-II

Paper Code: PPP.511

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 14 hours

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

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

Unit 2 20 hours

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

Unit 3 16 hours

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, memory effects, Mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzillic acid, Favorskii, Arndt-Eister syntheses, 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 and 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, antarasupra 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.

- 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 Insternational (P) Ltd., 5th edition, New Delhi.
- 5. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Insternational (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., (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. Organic Synthesis: The Disconnection Approach, John Wiley.
- 21. Cheng, Xue-Min; Corey, E.J. The Logic of Chemical Synthesis, John Wiley.

Course Tile: Phytochemical techniques and analysis

Paper Code: PPP.512

L	T	P	Credits	Marks
4	1	0	4	100

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

- 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, 6^{th} 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.
- 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 Tile: Basics of Drug Design and Drug Actions

Paper Code: PPP.513

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 12 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 Principal Physicochemical Parameters and Pharmacological Activity-Solubility, Partition Coefficient, Surface Activity, pKa, Ionisation, Stereochemical Factors, Bio-isosterism.

Unit 2 12 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

Discovery of Lead molecules and Drug Design: Natural products as lead structures in drug discovery. Structure pruning technique in lead modification e.g. morphine. Discovery of lead structure from natural harmones or neurotransmitters. Serendipitious discovery of leads e.g. Penicillin and Librium. Existing drugs as leads. Molecular graphics based lead discovery. Principles of design of agonists (e.g. Salbutamol), antagonists e.g. Cimitidine) and enzyme inhibitors (e.g. Captopril). Principles of prodrug design.

Unit 4 14 hours

Lead modification, SAR studies: 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 and 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.

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 5 20 hours

Combinatorial synthesis and chiral drugs: Introduction, Combinatorial approach. Combinatorial library, Solid phase synthesis, requirements, 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, High throughput screening Introduction to chiral drugs, Eutomer, distomer and eudesmic ratio. Pfeiffer's rule, Three point contact model. Synthesis of (S) naproxen, (S) propranolol, (S,S,S)-enalapril, (2S,3S)- diltiazem, indinavir sulfate.

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

Course Tile: Extraction and Isolation of Natural Products -

Practical

Paper	Code:	PPP.514
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L	Т	P	Credits	Marks
-	ı	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.

3.

Course Tile: Analyses and Molecular Modelling of Natural Products-Practical

L	T	P	Credits	Marks
-	-	4	2	50

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Paper	Coae:	PPP.	.515

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 Tile: Seminar

Paper Code: PPP.516

L	Т	P	Credits	Marks
-	-	4	2	50

Elective Courses

Course Tile: Chemistry of Natural Products

Paper Code: PPP.517

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 18 hours

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

Unit 2 18 hours

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

Unit 3 18 hours

Steroids: Occurrence, nomenclature, basic skeleton and stereochemistry, Structure determination and synthesis of cholesterol, partial synthesis of Testosterone, Progestrone, Biosynthesis of steroids.

Unit 4 9 hours

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

Porphyrins: Structure of haemoglobin.

Unit 5 9 hours

Glycosides: Occurrence, properties, classification, isolation, characterisation and chemical tests.

- 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 Tile: Advance Medicinal Chemistry

Paper Code: PPP.518

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 16 hours

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

Unit 2 18 hours

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

Unit 3 16 hours

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

Unit 4 22 hours

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

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

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

Course Tile: Green Chemistry

Paper Code: PPP.519

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1 22 hours

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

Unit 2 20 hours

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

Unit 3 18 hours

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

Unit 4 12 hours

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

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

Semester 3

Course Tile: Research Methodology

Paper Code: PPP.601

L	T	P	Credits	Marks
2	-	•	-	50

Unit 1 10 hours

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

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

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

Unit-2

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,

Good Laboratory Practices: Recent updates on good laboratory practices.

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.

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

Course Tile: Biostatistics

Paper Code: PPP.602

L	T	P	Credits	Marks
2	-	-	-	50

Unit 1 10 hours

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

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

Unit 2 5 hours

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

Unit 3 12 hours

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

Unit 4 9 hours

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

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

Course Tile: Biostatistics-Practical

Paper Code: PPP.603

L	T	P	Credits	Marks
	ı	4	2	50

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

Suggested Readings:

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

Course Tile: Mid-Term Evaluation of Thesis

Paper Code: PPP.604

L	Т	P	Credits	Marks
-	-	-	18	450

Semester 4

Course Tile: Medicinal Chemistry of Anticancer Agents

Paper Code: PPP.605

L	T	P	Credits	Marks
4	1	0	4	100

Unit 1

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

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

Unit 2

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

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

Unit 3

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

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

Unit 4

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

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

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

Course Tile: Thesis Evaluation and Viva Voce

Paper Code: PPP.606

L	T	P	Credits	Marks
-	-	-	20	500