Centre for Chemical and Pharmaceutical Sciences
Scheme of Programme
Ph.D. in Pharmaceutical Sciences

Duration of the Course: **3-5 Years**
Eligibility: **Master's degree in Pharmaceutical Sciences (Medicinal or Pharmaceutical Chemistry) with 55% marks from a recognized Indian or Foreign university**

SEMESTER 1

S. No.	Paper Code	Course Title	L	T	P	Cr	%Weightage				E
							A	B	C	D	
1	**PMC.701**	Research Methodology	2			2	10	15	15	10	50
2	**PMC.702**	Biostatistics	2			2	10	15	15	10	50
3	**PMC.703**	Computer Applications	2			2	10	15	15	10	50
*Opt any three of the following courses											
4	***PMC.704**	Natural Products in Drug Discovery and Development	4			4	25	25	25	25	100
5	***PMC.705**	Medicinal Chemistry of Nucleic Acids	4	-		4	25	25	25	25	100
6	***PMC.706**	Emerging Trends in Green Synthesis and Drug Discovery	4			4	25	25	25	25	100
7	***PMC.707**	Molecular Modeling and Molecular Dynamics	4			4	25	25	25	25	100
8	**PMC.708**	Seminar			-	2	-	-	-	-	50
		Total	18			20					500

A: <u>Continuous Assessment:</u> Subjective by enlarge
B: <u>Mid-Term Test-1:</u> Based on Objective Type & Subjective Type Test
C: <u>Mid-Term Test-2:</u> Based on Objective Type & Subjective Type Test
D: <u>End-Term Exam (Final):</u> Based on Objective Type Tests
E: Total Marks
L: Lectures   T: Tutorial   P: Practical   Cr: Credits

Course Tile: Research Methodology

Paper Code: PMC.701
Credits Hours: 2

L	T	P	Credits	Marks
2	-	-	-	50

Unit 1	10 hours

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

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

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

Unit-2	10 hours

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

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.

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

Course Tile: Biostatistics

Paper Code: PMC.702
Credits Hours: 2

L	T	P	Credits	Marks
2	-	-	-	50

Unit 1	10 hours

Overview of biostatistics: Difference between parametric and non-parametric statistics, Univariant and multivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.
Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Unit 2	5 hours

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

Unit 3	12 hours

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

Unit 4	9 hours

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

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

	L	**T**	**P**	**Credits**	**Marks**
Course Tile: Computer Applications	2	0	0	2	50

Course Tile: Computer Applications
Paper Code: PMC.703
Credits Hours: 2

Unit 1	**18 hours**

Fundamentals of computers: Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean algebra.
Application software: Spreadsheet applications, Word-processing applications, Presentation applications, Internet browsers, Reference Management, and Image processing applications.

Unit 2	**18 hours**

Computer language: Basic DOS commands, AutoHotKey scripting language, HTML and basic structure of a webpage, Designing websites.
World wide web: Origin and concepts, Latency and bandwidth, Searching the internet, Advanced web-search using Boolean logic, Cloud computing.

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

Course Tile: Natural Products in Drug Discovery and Development
Paper Code: PMC.704
Credits Hours: 4

L	T	P	Credits	Marks
4	-	-	4	100

Unit 1	**12 hours**

Prospects of Natural Products research in the 21st Century: - Introduction, use of natural products in traditional medicines, potential of natural products, Natural products in drug discovery and development. Use of herbal remedies and the potential of drug development from natural products and novel drug templates: paclitaxel, podophyllotoxin, artimisinin etc.

Unit 2	**12 hours**

Recent development in the research on naturally occurring flavonoids: - Introduction, Recently reported flavonoids, flavonoids as drug candidates, Biological and Pharmacological activities of flavonoids (Antioxidant activity, cyto-toxic activity, anticancer and anti-turmeric activities, cardio protective effect, anti-microbial activity).

Unit 3	**12 hours**

Glycodrugs: - A new window for chemo-diversity and drug discovery from natural products-Introduction, Antibiotics, Anti-cancers and Anesthetics.

Unit 4	**12 hours**

Alkaloids: - Recent developments in pharmacological, biological and medicinal aspects-Introduction, Antimicrobial activity, antioxidant and anti-inflammatory activities of alkaloids.

Unit 5	**12 hours**

Terpenoids: - Old secondary metabolites with new therapeutic properties- Introduction, general biosynthesis of terpenoids, Ecological role of terpenoids and terpenoids in herbal medicines.
Essential Oils:- Introduction, manufacturing process, processing of essential oils, uses of essential oils and composition of essential oils, Pharmacological applications.

Unit 6	**12 hours**

Semi-synthesis of natural drug analogues for their bioavailability specially focus on anticancer and anti-diabetic molecules, green approaches used for increasing bioavailability and biological activity

Suggested references

1. Bhat, S.V.; Nagasampagi, B.A.; Meenakshi, S. (2009) Natural Product Chemistry & Applications. Publisher: Narosa Publishing House, New Delhi.
2. Finar, I.L. (2006) Organic Chemistry: Stereochemistry and the Chemistry of Natural Products. 5th edn, Dorling Kindersley (India) Pvt. Ltd., New Delhi.
3. Bhat, S.V.; Nagasampagi, B.A.; Sivakumar, M. (2005) Chemistry of Natural Products. Publisher: Narosa Publishing House, New Delhi.
4. Butler, M.S. (2005) Natural products to drugs: natural product derived compounds in clinical trials. Natural Product Report, 22, 162-195

Course Tile: Medicinal Chemistry of Nucleic Acids
Paper Code: PMC.705
Credits Hours: 4

L	T	P	Credits	Marks
4	-	-	4	100

Unit 1   **18 hours**

Nucleic acids: Introduction, central dogma, biosynthesis, structure (conformation, size, shape, bending, supercoiling etc.) and functions (transcription, post transcriptional modifications and translations) and damage and repair. Genetic polymorphism.

Unit 2   **18 hours**

Protein-nucleic acid interactions: proteins involved in the biosynthesis of nucleic acids, enzymes in replications, transcription and translation. Damage and repair enzymes and epigenetic factors (HDAC/nucleosomes/HATs/MTs).

Unit 3   **18 hours**

Drug design and synthesis: Drugs targeting nucleic acids conformations, drugs targeting associated proteins, drugs mimicking, drugs targeting replication/transcription/translation and the proteins mentioned in unit 2. Drugs affecting gene expression (kinase inhibitors etc.)
The SAR and *in silico* and pharmacokinetic approaches: to be discussed wherever possible in above mentioned topics.

Unit 4   **18 hours**

Nucleic acids in R&D and diseases: Diseases associated with nucleic acids (such as SNPs and chromosomal inversions etc.). Anti-nucleic acid therapies and naturally occurring small antisense RNAs (Si/micro RNA). Therapies of nucleic acids in stem cells. Vehicles mediated targeted delivery.

Suggested Readings:
1. Zhang, L.-H., Xi, Z., Chattopadhyaya, J. (2011), *Medicinal Chemistry of Nucleic Acids*, Wiley, 1 edition.
2. Mayer, G. (2010), *The Chemical Biology of Nucleic Acids*, Wiley, 1 edition.
3. Bloomfield, V. A., Crothers, D. M., Tinoco, I., Hearst, J. E., Wemmer, D. E., Killman, P. A., Turner, D. H. (2000) *Nucleic Acids: Structures, Properties, and Functions,* University Science Books; 1 edition.
4. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., 7th edition, Philadelphia.
5. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, 6th edition, Philadelphia.
6. Neidle, S. (2007), *Principles of Nucleic Acid Structure*, Academic Press; 1 edition.
7. Blackburn, G. M., Gait, M. J., Loakes, D., Williams; D. (2006), *Nucleic Acids in Chemistry and Biology*, Royal Society of Chemistry; 1 edition.
8. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd Edition, London.
9. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3rd edition, New York.
10. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4th edition. UK.

11. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
12. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier), 3rd edition.
13. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery*, John Wiley and Sons, New York.

Course Tile: Emerging Trends in Green Synthesis and Drug Discovery
Paper Code: PMC.706
Credits Hours: 4

L	T	P	Credits	Marks
4	-	-	4	100

Unit 1	**18 hours**

Microwave Assisted Organic synthesis (MAOS): Heating effects of microwaves: (i) Dipolar polarization and (ii) Ionic conduction, Synthesis of target molecules under solventless conditions and on solid support, Microwave and stereoselectivity, Recent advancement in aqueous reaction conditions and microwave.

Unit 2	**18 hours**

Synthesis of Bioactive molecules using Ionic Liquids: Ionic liquids as green solvents, Replacement of volatile organic solvents and environmental impact, Ionic liquids as catalyst, Designer solvents, Ionic liquids and asymmetric synthesis.

Unit 3	**18 hours**

Synthesis of important bioactive molecules: Plants of North India (mainly Punjab, Himachal Pradesh, Haryana and Rajasthan), Redundant nature derived products and their value addition, Chemical modification to bioactive molecules, Synthesis of paclitaxel from baccatin, Innocuous and agro based starting material.

Unit 4	**18 hours**

Recent Trends in Drug Discovery: Computer in drug designing, Natural product based drug design, Identification of target molecules, Lead candidate and lead optimization, Ligands with multi receptor affinity profile, Diversity oriented synthesis in drug discovery, Nano drug delivery systems.

Suggested Reading:
1. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson, 4th edition, UK.
2. Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical*. Oxford University Press, 1st edition, US.
3. Paul, M.D. (**1997**) *Medicinal Natural Products: A Biosynthetic Approach*, John Wiley & Sons., New York.
4. Walton, N.J., Brown, D.E. (**1999**) *Chemicals from Plants: Perspectives on Plant Secondary Products*, Imperial College Press, London.
5. Gang, D.R., Wang, J., Dudareva, N., Nam, K.H., Simon, J.E., Lewinsohn, E., Pichersky, E. *Plant Physiol*., **2001**, *125*, 539.
6. Rubenstein, K., (2009), Medicinal Chemistry for Drug Discovery: Significance of Recent Trends, Insight Pharma Reports.
7. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd Edition, London.
8. Unique versatility of Ionic liquids as clean and efficient decarboxylation catalyst: A metal and quinoline free paradigm towards synthesis of Indoles, Styrenes, Stilbenes and Arene derivatives under microwave in aqueous condition, Abhishek Sharma, Rakesh Kumar, Naina Sharma, Vinod Kumar and Arun K. Sinha, *Adv. Synth. Catal.,* 2008, 350, 2910-2920.

9. A Chemoselective Hydrogenation of the Olefinic Bond of α, β-Unsaturated Carbonyl Compounds in Aqueous Medium Under Microwave Irradiation; Anuj Sharma, Vinod Kumar and A. K Sinha, *Adv. Synth. Catal.,* 2006, 348, 354-360.

10. Remarkable Synergism in Methylimidazole-Promoted Decarboxylation of Substituted Cinnamic acids in basic water medium under Microwave Irradiation: A Clean Synthesis of Hydroxylated (*E*)-Stilbenes; Vinod Kumar, Abhishek Sharma, Anuj Sharma and Arun K. Sinha, *Tetrahedron*, 2007, *63,* 7640-7646.

11. Microwave-assisted Mild Conversion of Natural Dihydrotagetone into 5-Isobutyl-3-methyl-4,5-dihydro-2(3H)-furanone: an Analogue of Whisky Lactone; Arun K. Sinha, Bhupender P. Joshi, Anuj Sharma, Vinod Kumar and Ruchi Acharya, *Aust. J. Chem.*, 2007, 60, 124-127

Course Tile: Molecular Modeling and Molecular Dynamics
Paper Code: PMC.707
Credits Hours: 4

L	T	P	Credits	Marks
4	-	-	4	100

Unit 1	**18 hours**

Computational Chemistry: Concepts of Computational Chemistry: Börn-Oppenheimer approximations, Application of Hartree-Fock equations to molecular systems, approximate molecular orbital theories, Semi-empirical methods. Macro-molecular Force Fields, Solvation, Long range forces.

Unit 2	**18 hours**

Molecular Mechanics: General features, Bond stretching, Angle bending, Improper torsions, Out-of-plane bending, Cross terms, Non-bonded interactions, Ramachandran diagram, point charges, calculation of atomic charges, Polarization, Van der Waals interactions, Hydrogen bond interactions, Water models, Force field, all atoms force field and united atom force field.

Unit 3	**18 hours**

Energy minimization: Steepest descent, conjugate gradient–Derivatives, First order steepest decent and conjugate gradients. Second order derivatives Newton-Raphson, Minima, maxima saddle points and convergence criteria; non derivatives minimization methods, the simplex, sequential univariative.

Unit 4	**18 hours**

Simulation methods: Newton's equation of motion, equilibrium point, radial distribution function, MD methodology, Periodic box, Solvent access, Equilibration,Cutoffs, algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzmann velocity, timesteps, duration of the MD run, Starting structure, analysis of MD job, uses in drug designing, ligand-protein interactions.

Recommended Books:
1. A. R. Leach, Molecular Modelling Principles and Applications, Prentice Hall (2001).
2. H. Fenniri, Combinatorial Chemistry–A practical Approach, Oxford University Press, UK (2000).
3. D. Lednicer, Strategies for Organic Drug Discovery Synthesis and Design; Wiley International Publishers (1998).
4. E. M. Gordon, J. F Kerwin, Combinatorial Chemistry and Molecular Diversity in Drug Discovery, Wiley-Blackwell Publishers (1998).
5. D. Frenkel, B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, Elsevier (2012).
6. D. C. Rapaport, The Art of Molecular Dynamics Simulation, Cambridge University Press (2004).