CENTRAL UNIVERSITY OF PUNJAB



Doctor of Philosophy (Medicinal Chemistry)

Session – 2021 Course work

Department of Pharmaceutical Sciences and Natural Products

Graduate attributes

The Ph.D. program in Medicinal Chemistry would provide outstanding education in drug discovery through multidisciplinary training in synthetic organic chemistry, natural products, drug design, molecular metabolism and chemical toxicology, and mechanisms of drug action in preparation for careers in industry, government, or institutions of higher learning. The program would also help students start an industry start-up and become great teachers and independent scientists.

Course Structure

SEMESTER 1 (Course Work)

S. No.	Paper Code	Course Title			P	Cr	
1	CMC.701	Research Methodology & Biostatistics			0	4	
2	CMC.703	Computer Applications	2	0	0	2	
3	CMC.751	Research and Publication Ethics	2	1	1	2	
4	CMC.752	Teaching Assistantship	0	0	2	1	
5	UNI.753	Curriculum, Pedagogy and Evaluation	1	0	0	1	
6	CMC.709	Seminar	0	0	0	2	
*Opt fo	*Opt for any one of the following courses						
7	*CMC.704	Natural Products in Drug Discovery and Development: Recent Advances	4	0	0	4	
8	*CMC.705	Recent Advances in Medicinal Chemistry of Nucleic Acids	4	0	0	4	
9	*CMC.706	Emerging Trends in Green Synthesis and Drug Discovery			0	4	
10	*CMC.707	Trends in Molecular Modelling for Drug Design	4	0	0	4	
		Total	16			16	

^aTo be offered by School of Education

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

^{**}Any other relevant course offered by a faculty member of the same department or another department/School-To be decided by the respective supervisor.

Course Title: Research Methodology &

Biostatistics

Paper Code: CMC.701

L	T	P	Credits
4	0	0	4

Learning Outcomes:

After successfully completing this course, the learner would be able to:

- 1. Select and define an appropriate research problem and parameter
- 2. Design and set the objectives based on the literature search.
- 3. Gain the knowledge of protecting the research work through patent or copyright or trademarks.
- 4. Learn basic descriptive and inferential statistics, including the concepts and principles of research design and statistical inference.
- 5. Perform and interpret descriptive and inferential statistical techniques, including the construction of tables and graphs, t-tests, Chi-square tests, and regression analysis.
- 6. Use appropriate software packages to solve analytical problems.

Unit 1 15 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.

Bibliographic index and research quality parameters- citation index, impact factor, h index, i10 index, etc. Research engines such as google scholar, Scopus, web of science, etc.

Intellectual Property Rights: Intellectual Property, intellectual property protection

(IPP) and intellectual property rights (IPR), WTO (World Trade Organization), WIPO (World Intellectual Property Organization), GATT (General Agreement on Tariff and Trade), TRIPs (Trade-Related Intellectual Property Rights), TRIMS (Trade-Related Investment Measures) and GATS (General Agreement on Trades in Services), Nuts and Bolts of Patenting, Technology Development/Transfer Commercialization Related Aspects, Ethics and Values in IP.

Unit 2 15 hours

Technical writing: Technical & Scientific writing - theses, technical papers, reviews, electronic communication, research papers, etc., Poster preparation and Presentation and Dissertation. Reference Management using various

softwares such as Endnote, reference manager, Ref works, etc. Communication skills – defining communication; type of communication; techniques of communication, etc.

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

Plagiarism: Plagiarism, definition, Search engines, regulations, policies and documents/thesis/manuscripts checking through softwares, Knowing and Avoiding Plagiarism during documents/thesis/manuscripts/scientific writing

Unit-3 15 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, stem and leaf plot, pie chart.

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-4 15 hours

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

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, Kruskal-Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks.

Suggested Readings:

- 1. Gupta, S. (2008). Research methodology and statistical techniques. New Delhi: Deep & Deep Publications (p) Ltd.
- 2. Kothari, C. R. (2008.) *Research methodology(s)*. New Delhi: New Age International (p) Limited.
- 3. Best J. W., Khan J. V., Jha, A.K. (2014). *Research in Education*. India: Pearson Education India.
- 4. National Research Council. (2014). Safe science: promoting a culture of safety in academic chemical research. Washington DC: National Academic Press.

- 5. Copyright Protection in India [website: http:copyright.gov.in].
- 6. World Trade Organization [website: www.wto.org].
- 7. Wadedhra B.L. (2006). Law Relating to Patents, Trademarks, Copyright Design and Geographical Indications. New Delhi: Universal Law Publishing.
- 8. Creswell, D., Creswell, J. W. (2018). *Research Design: Qualitative, Quantitative, and Mixed Methods Approaches*. SAGE Publications, Inc.
- 9. Gookin, D. (2007). *MS Word for Dummies*. Hoboken, NJ: Wiley Publishing, Inc.
- 10. Harvey, G. (2007). MS Excel for Dummies. Hoboken, NJ: Wiley Publishing, Inc.
- 11. Sinha, P.K. Sinha, P. (2010). Computer Fundamentals. India: BPB Publications.
- 12. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials*.. Canada: Decker Inc.
- 13. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, New York:W.H. Freeman and Company. Bolton, S., & Bon, C. (2009). *Pharmaceutical statistics: practical and clinical applications*. Boca Raton: CRC Press.

The following are some of the modes of classroom transaction

- 1) Lecture
- 2) Demonstration
- 3) Lecture cum demonstration

Course Title: Computer Applications

L	T	P	Credits
2	0	0	2

Paper Code: CMC.702 Learning Outcomes:

After successfully completing this course, learner would be able to:

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

Unit 1 8 hours

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

Unit 2 7 hours

MS Word (Word Processing, Creating and Saving Documents, Text Formatting, Tables, Document Review Option, Inserting Table of Contents), Power point, Excel Sheet.

Unit 3 7 hours

Scientific information retrieval and web browsing: Introduction to various search engines such as Protein Data Bank, PubMed, NISCAIR, ACS, RSC, Elsevier, SciFinder, Google Scholar, Google patent, Espacenet, Beilstein databases, etc.

Unit 4 8 hours

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. Sinha, P. (2010). *Computer Fundamentals*. India: BPB Publications.
- 2. Goel, A., Ray, S. K. (2012). *Computers: Basics and Applications*. India: Pearson Education India.
- 3. Microsoft Office Professional 2013 Step by Step. Retrieved from https://ptgmedia.pearsoncmg.com/images/9780735669413/samplepages/97807356694 13.pdf
- 4. Gookin, D. (2007). *MS Word for Dummies*. Hoboken, NJ: Wiley Publishing, Inc.
- 5. Harvey, G. (2007). *MS Excel for Dummies*. Hoboken, NJ: Wiley Publishing, Inc.
- 6. Bott, E., Siechert, C., & Stinson, C. (2010). *Windows 7 inside out*. Washington: Microsoft Press.

The following are some of the modes of classroom transaction

- 1) Lecture
- 2) Demonstration
- 3) Lecture cum demonstration

Course Code: CMC.751

Course Title: Research and Publication Ethics

L	Т	Р	Credits
2	0	0	2

Total Hours: 30

Unit I Philosophy and Ethics

3 hours

- Introduction to Philosophy : definition, nature and scope, content, branches
- Ethics : definition, moral philosophy, nature of moral judgements and reactions

Unit II Scientific Conduct

5 hours

- Ethics with respect to science and research
- Intellectual honesty and research integrity
- Scientific misconducts : Falsification, Fabrication, and Plagiarism (FFP)
- Redundant publications : duplicate and overlapping publications, salami slicing
- Selective reporting and misrepresentation of data

Unit III: Publication Ethics

7 hours

- Publication ethics : definition, introduction and importance
- Best practices/ standards setting initiatives and guidelines: COPE, WAME, etc.
- Conflicts of interest
- Publication misconduct : definition, concept, problems that lead to unethical behaviour and vice versa, types
- Violation of publication ethics, authorship and contributor ship
- Identification of publication misconduct, complaints and appeals
- Predatory publishers and journals

Unit IV Open Access publishing

4 hours

- Open access publications and initiatives
- SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
- Software tool to identify predatory publication developed by SPPU
- Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer, Journal Suggester etc.

Unit V Publication Misconduct

4 hours

- Group Discussions: Subject specific ethical issues, FFP, authorship; conflicts of interest; complaints and appeals: examples and fraud from India and abroad
- Software tools: Use of plagiarism software like Turnitin, Urkund and other open source software tools

Unit IV Databases and Research Metrics

7 hours

- Databases: Indexing databases; Citation database: Web of Science, Scopus etc.
- Research Metrics: Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score; Metrics: h-index, g-index, i10 index, almetrics

Course Code: CMC.752

Course Title: TEACHING ASSISTANTSHIP

L	T	P	Credit
0	0	2	1

Total Hours: 30

Learning Outcome:

At the end of this skill development course, the scholars shall be able to familiarize themselves with the pedagogical practices of effective class room delivery and knowledge evaluation system

1. manage large and small classes using appropriate pedagogical techniques for different types of content

Activities and Evaluation:

- The scholars shall attend Master degree classes of his/her supervisor to observe the various transaction modes that the supervisor follows in the class room delivery or transaction process one period per week.
- The scholars shall be assigned one period per week under the direct supervision of his/her supervisor to teach the Master degree students adopting appropriate teaching strategy(s).
- The scholars shall be involved in examination and evaluation system of the Master degree students such as preparation of questions, conduct of examination and preparation of results under the direction of the supervisor.
- At the end of the semester, the supervisor shall conduct an examination of teaching skills learned by the scholar as per the following evaluation criteria:
- The scholars shall be given a topic relevant to the Master degree course of the current semester as his/her specialization to prepare lessons and deliver in the class room before the master degree students for one hour (45 minutes teaching + 15 minutes interaction).
- The scholars shall be evaluated for a total of 50 marks comprising content knowledge (10 marks), explanation and demonstration skills (10

marks), communication skills (10 marks), teaching techniques employed (10 marks), and classroom interactions (10).

Course Code: UNI.753

Course Title: CURRICULUM, PEDAGOGY AND EVALUATION_____

L	T	Р	Credit
1	0	0	1

Total Hours: 15

Learning outcomes:

After completion of the course, scholars shall be able to:

- analyze the principles and bases of curriculum design and development
- examine the processes involved in curriculum development
- develop the skills of adopting innovative pedagogies and conducting students' assessment
- develop curriculum of a specific course/programme

Course Content

Unit I Bases and Principles of Curriculum

4 hours

- 1. Curriculum: Concept and Principles of curriculum development, Foundations of Curriculum Development.
- 2. Types of Curriculum Designs- Subject centered, learner centered, experience centered and core curriculum. Designing local, national, regional and global specific curriculum. Choice Based Credit System and its implementation.

Unit II Curriculum Development

4 hours

- 1. Process of Curriculum Development: Formulation of graduate attributes, course/learning outcomes, content selection, organization of content and learning experiences, transaction process.
- 2. Comparison among Interdisciplinary, multidisciplinary and transdisciplinary approaches to curriculum.

Unit III Curriculum and Pedagogy

3 hours

- 1. Conceptual understanding of Pedagogy.
- 2. Pedagogies: Peeragogy, Cybergogy and Heutagogy with special emphasis on Blended learning, Flipped learning, Dialogue, cooperative and collaborative learning
- 3. Three e- techniques: Moodle, Edmodo, Google classroom

Unit IV Learners' Assessment

4 hours

1. Assessment Preparation: Concept, purpose, and principles of preparing objective and subjective questions.

- 2. Conducting Assessment: Modes of conducting assessment offline and online; use of ICT in conducting assessments.
- 3. Evaluation: Formative and Summative assessments, Outcome based assessment, and scoring criteria.

Transaction Mode

Lecture, dialogue, peer group discussion, workshop

Evaluation criteria

There shall be an end term evaluation of the course for 50 marks for duration of 2 hours. The course coordinator shall conduct the evaluation.

Suggested Readings

- Allyn, B., Beane, J. A., Conrad, E. P., & Samuel J. A., (1986). Curriculum Planning and Development. Boston: Allyn & Bacon.
- Brady, L. (1995). Curriculum Development. Prentice Hall: Delhi. National Council of Educational Research and Training.
- Deng, Z. (2007). Knowing the subject matter of science curriculum, Journal of Curriculum Studies, 39(5), 503-535. https://doi.org/10.1080/00220270701305362
- Gronlund, N. E. & Linn, R. L. (2003). Measurement and Assessment in teaching.
- Singapore: Pearson Education
- McNeil, J. D. (1990). Curriculum: A Comprehensive Introduction, London: Scott,
- Foreman/Little
- Nehru, R. S. S. (2015). Principles of Curriculum. New Delhi: APH Publishing Corporation.
- Oliva, P. F. (2001). Developing the curriculum (Fifth Ed.). New York, NY: Longman
- Stein, J. and Graham, C. (2014). Essentials for Blended Learning: A Standards-Based Guide. New York, NY: Routledge.

Web Resources

- https://www.westernsydney.edu.au/__data/assets/pdf_file/0004/46709
 5/Fundamentals_of_Blended_Learning.pdf
- https://www.uhd.edu/academics/university-college/centers-offices/teaching-learningexcellence/Pages/Principles-of-a-Flipped-Classroom.aspx
- http://leerwegdialoog.nl/wp-content/uploads/2018/06/180621-Article-The-BasicPrinciples-of-Dialogue-by-Renate-van-der-Veen-and-Olga-Plokhooij.pdf

Course Title: Seminar Paper Code: CMC.704S

Learning Outcome: The student will be able to

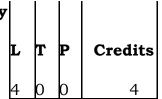
☐ Elucidate and demonstrate the technical writing and present the problem in hand, highlighting the various ways the problem is addressed in the

literature.

L	T	P	Credits
О	0	0	2

Course Title: Natural Products in Drug Discovery and Development: Recent Advances

Paper Code: CMC.705



Learning Outcomes:

After successfully completing this course, learner would be able to:

- 1. Be familiar with the prospects of natural products
- 2. Gain function of natural products in living organisms, their biosynthesis and medicinal properties

Unit 1 15 h

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

Unit 2 15 h

Recent development in the research on naturally occurring polyphenolic compounds: - Introduction, recently reported flavonoids, flavonoids as drug candidates, Biological and Pharmacological activities of flavonoids (Antioxidant activity, cytotoxic activity, anticancer and anti-microbial activity), Biosynthetic pathway.

Unit 3 15 h

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

Unit 4 15 h

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.

Steroids: Determination and synthesis of cholesterol, partial synthesis of Testosterone and Progesterone, Chemical tests for steroids, Medicinal applications of steroids.

Suggested Readings:

- 1. Brahamchari, G. (2009). *Natural Product: Chemistry, Biochemistry and Pharmacology*. New Delhi, India: Narosa Publishing House.
- 2. Cseke, L.J. (2009). *Natural Products from plants*. US: CRC Press, Taylor and Francis.
- 3. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. UK: Willey & Sons.
- 4. Peterson, F., Amstutz, R. (2008). *Natural Compounds as drugs:* Vol 2. Birkhäuser Basel.
- 5. Thomson, R.H. (2008). *The Chemistry of Natural Products*, Springer, Netherlands: Springer Netherlands.
- 6. Singh, J., Ali, S. M., Singh, J. (2010) *Natural Products Chemistry*. India: Pragati Books.
- 7. Xu, R., Ye, Y., Zhao, W. (2011). *Introduction to Natural Products Chemistry*. Beijing, China: CRC Press.
- 8. Rehman, A., (2015). Studies in Natural Products Chemistry: Vol 45. Elsevier Books.
- 9. Mandal, S., Mandal, V., Konishi, T. (2018). *Natural Products and Drug Discovery*. Elsevier.

The following are some of the **modes of classroom transaction**

- 1) Lecture
- 2) Demonstration
- 3) Lecture cum demonstration
- 4) Video

Course Title: Recent Advances in Medicinal

Chemistry of Nucleic Acids

L	Т	P	Credits
4	0	0	4

Paper Code: CMC.706 Learning outcomes:

After successfully completing this course, learner would be able to:

- 1. Design of new inhibitors of nucleic acids
- 2. Drug targets in diseases like cancer and others.

Unit 1 15 h

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 15 h

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

Unit 3 15 h

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 the abovementioned topics.

Unit 4 15 h

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*. New York, USA: A John Wiley & Sons, Inc., Publication.
- 2. Mayer, G. (2010). *The Chemical Biology of Nucleic Acids*, New York, USA: A John Wiley & Sons, Inc., Publication.
- 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.
- 4. Beale, J. M., Block, J.H. (2011). Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry. Philadelphia: J. Lippincott Co.
- 5. Foye, W. C. (2008). *Principles of Medicinal Chemistry*. Philadelphia: Lea and Febiger.
- 6. Neidle, S. (2007). Principles of Nucleic Acid Structure. Academic Press.
- 7. Blackburn, G. M., Gait, M. J., Loakes, D., Williams; D. (2006). *Nucleic Acids in Chemistry and Biology*. Royal Society of Chemistry.
- 8. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*. London: Royale Society of Chemistry.
- 9. Nogardy, T., Weaver, D.F. (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*. New York: Oxford University Press.
- 10. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*. UK Oxford University Press.
- 11. Singh, H., Kapoor, V.K. (2012). *Medicinal and Pharmaceutical Chemistry*. Delhi, India: Vallabh Prakashan.
- 12. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*. Academic Press (Elsevier).
- 13. Wolff, M E, Ed. (2010). *Burger's Medicinal Chemistry and Drug Discovery*. New York, USA: John Wiley and Sons.

The following are some of the modes of classroom transaction

- 1) Lecture
- 2) Demonstration
- 3) Lecture cum demonstration
- 4) Video

Course Title: Emerging Trends in Green Synthesis and Drug Discovery

L T P Credits

Paper Code: CMC.707 Learning outcomes:

4	0	0	4

After successfully completing this course learner would be able to:

- 1. Learn and draw the mechanism of microwave assisted organic transformation
- 2. Conduct ionic liquids, solid supported organic reactions under MW and conventional conditions
- 3. Utilize metal and organocatalysts for various C-C and C-N bond formation reactions Apply recent tools in drug discovery and developments

Unit 1 15 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 15 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 15 hours

Developments in metal catalysis and organocatalysis

New developments in the palladium catalyzed chemistry for C-C bond formation reaction, copper catalyzed C-N bond formation reactions, metal catalyzed reactions under microwave conditions, Solid supported reactions, Organic catalytic systems

Unit 4 15 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 Readings:

1. Mann, F.G., and Saunders, B.C. (2009). *Practical organic chemistry*, UK: Pearson.

- 2. Anastas, P.T., Warner, J. C. (2000). *Green chemistry, Theory and Practical*. US: Oxford University Press.
- 3. Paul, M.D. (1997). *Medicinal Natural Products: A Biosynthetic Approach*. New York: John Wiley & Sons.
- 4. Walton, N.J., Brown, D.E. (1999). *Chemicals from Plants: Perspectives on Plant Secondary Products*. London, UK: Imperial College Press.
- 5. Gang, D.R., Wang, J., Dudareva, N., Nam, K.H., Simon, J.E., Lewinsohn, E., Pichersky, E. (2001). *Plant Physiol.* 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*, London: Royale Society of Chemistry.
- 8. Sharma, A., Kumar, R., Sharma, N., Kumar, V., & Sinha, A. K. (2008). Unique Versatility of Ionic Liquids as Clean Decarboxylation Catalyst Cum Solvent: A Metal- and Quinoline- Free Paradigm towards Synthesis of Indoles, Styrenes, Stilbenes and Arene Derivatives under Microwave Irradiation in Aqueous Conditions. Advanced Synthesis & Catalysis, 350(18), 2910-2920.
- 9. Sharma, A., Kumar, V., & Sinha, A. K. (2006). A Chemoselective Hydrogenation of the Olefinic Bond of a, β Unsaturated Carbonyl Compounds in Aqueous Medium under Microwave Irradiation. Advanced Synthesis & Catalysis, 348(3), 354-360.
- 10. Kumar, V., Sharma, A., Sharma, A., & Sinha, A. K. (2007). Remarkable synergism in methylimidazole-promoted decarboxylation of substituted cinnamic acid derivatives in basic water medium under microwave irradiation: a clean synthesis of hydroxylated (E)-stilbenes. Tetrahedron, 63(32), 7640-7646.
- 11. Sinha, A. K., Joshi, B. P., Sharma, A., Kumar, V., & Acharya, R. (2007). *Microwave-assisted mild conversion of natural dihydrotagetone into 5-isobutyl-3-methyl-4*, *5-dihydro-2 (3H)-furanone, an analogue of whisky lactone*. Australian journal of chemistry, 60(2), 124-127.

The following are some of the **modes of classroom transaction**

- 1) Lecture
- 2) Demonstration
- 3) Lecture cum demonstration

Course Title: Trends in Molecular Modelling for

Drug Design

Paper Code: CMC.708 Learning outcomes:

4 0 0 4	L	T	P	Credits
	4	0	0	4

After successfully completing this course, learner would be able to:

- 1. How a slight change in substituents affect the biological activity of drugs?
- 2. How molecular modelling can increase efficiency?
- 3. Pharmacophore and receptor-based rational drug design.

Unit 1 15 hours

QSAR: Introduction, history, applications, various descriptors used in QSARs: lipophilicity, electronic, stearic based descriptors. Regression analysis, significance and validity of QSAR regression equations, case study – on pyranenamine, partial least squares (PLS) analysis, multi linear regression analysis. Use of genetic algorithms, neural networks and principle components analysis in the QSAR equations.

Unit 2 15 hours

2D QSAR: 2D QSAR techniques like Free-Wilson Analysis, Ban-Fujita modification, Topliss operational scheme, Craig Plot, Cluster Analysis and Hansch analysis and their applications.

Unit 3 15 hours

3D QSAR: COMFA – 3D QSAR techniques like Comparative molecular field analysis, CoMSIA- Comparative Molecular Similarity Indices Analysis, CoMSA-Comparative Molecular Surface Analysis, SOMFA - Self-organizing molecular field analysis and their applications.

Unit 4 15 hours

Virtual Screening and Molecular docking: Drug likeness screening, Concept of pharmacophore mapping and pharmacophore-based Screening, **Molecular docking:** Rigid docking, flexible docking, manual docking; Docking based screening, *De novo* drug design.

Suggested Readings:

- 1. Thomas, G. (2007). *Medicinal Chemistry-An Introduction.*, New York, USA: John Wiley and sons Ltd.
- 2. Nogrady, T., Weaver, D. F. (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach.*, New York, USA: OXFORD University Press Inc.
- 3. Krogsgaard-Larsen, P., Strogaard, K., Madsen, U. (2009). *Textbook of Drug Design and Discovery*, United States: CRC Press.
- 4. Silverman, R. B., Holladay, M. W. (2014). *Organic Chemistry of the Drug Design and Drug* Action. Waltham, USA: Academic Press.
- 5. Foye, W. C. (2008). *Principles of Medicinal Chemistry*. Philadelphia: Lea and Febiger.
- 6. Delgado, J. N. and Remers, W. A., Ed. (2010) Wilson and Gisvolds Text book of Organic and Pharmaceutical Chemistry. Philadelphia: J. Lipincott Co.
- 7. Patrick, G. L. (1995). *An introduction to Medicinal Chemistry*. New York, USA: Oxford University Press Inc.

The following are some of the modes of classroom transaction

- 1) Lecture
- 2) Demonstration
- 3) Lecture cum demonstration
- 4) Video
- 5) Self-learning

Course Title: TEACHING ASSISTANTSHIP

 L
 T
 P
 Credit

 0
 0
 2
 1

Total Hours: 30

Learning Outcome:

At the end of this skill development course, the scholars shall be able to

- (1) familiarize themselves with the pedagogical practices of effective class room delivery and knowledge evaluation system
- (2) manage large and small classes using appropriate pedagogical techniques for different types of content

Activities and Evaluation:

- The scholars shall attend Master degree classes of his/her supervisor to observe the various transaction modes that the supervisor follows in the class room delivery or transaction process one period per week.
- The scholars shall be assigned one period per week under the direct supervision of his/her supervisor to teach the Master degree students adopting appropriate teaching strategy(s).
- The scholars shall be involved in examination and evaluation system of the Master degree students such as preparation of questions, conduct of examination and preparation of results under the direction of the supervisor.
- At the end of the semester, the supervisor shall conduct an examination of teaching skills learned by the scholar as per the following **evaluation criteria**:
- The scholars shall be given a topic relevant to the Master degree course of the current semester as his/her specialization to prepare lessons and deliver in the class room before the master degree students for one hour (45 minutes teaching + 15 minutes interaction).
- The scholars shall be evaluated for a total of 50 marks comprising *content knowledge* (10 marks), *explanation and demonstration skills* (10 marks), *communication skills* (10 marks), *teaching techniques employed* (10 marks), and classroom interactions (10).

Course Title: CURRICULUM, PEDAGOGY AND EVALUATION

L	T	P	Credit
1	0	0	1

Course Code: XXXX

Learning outcomes:

After completion of the course, scholars shall be able to:

- analyze the principles and bases of curriculum design and development
- examine the processes involved in curriculum development
- develop the skills of adopting innovative pedagogies and conducting students' assessment
- develop curriculum of a specific course/programme

Course Content

Unit I Bases and Principles of Curriculum

4 hours

Total Hours: 15

- 1. Curriculum: Concept and Principles of curriculum development, Foundations of Curriculum Development.
- 2. Types of Curriculum Designs- Subject centered, learner centered, experience centered and core curriculum. Designing local, national, regional and global specific curriculum. Choice Based Credit System and its implementation.

Unit II Curriculum Development

4 hours

- 1. Process of Curriculum Development: Formulation of graduate attributes, course/learning outcomes, content selection, organization of content and learning experiences, transaction process.
- 2. Comparison among Interdisciplinary, multidisciplinary and trans-disciplinary approaches to curriculum.

Unit III Curriculum and Pedagogy

3 hours

- 1. Conceptual understanding of Pedagogy.
- 2. Pedagogies: Peeragogy, Cybergogy and Heutagogy with special emphasis on Blended learning, Flipped learning, Dialogue, cooperative and collaborative learning
- 3. Three e- techniques: Moodle, Edmodo, Google classroom

Unit IV Learners' Assessment

4 hours

- 1. Assessment Preparation: Concept, purpose, and principles of preparing objective and subjective questions.
- 2. Conducting Assessment: Modes of conducting assessment offline and online; use of ICT in conducting assessments.
- 3. Evaluation: Formative and Summative assessments, Outcome based assessment, and scoring criteria.

Transaction Mode

Lecture, dialogue, peer group discussion, workshop

Evaluation criteria

There shall be an end term evaluation of the course for 50 marks for duration of 2 hours. The course coordinator shall conduct the evaluation.

Suggested Readings

- Allyn, B., Beane, J. A., Conrad, E. P., & Samuel J. A., (1986). *Curriculum Planning and Development*. Boston: Allyn & Bacon.
- Brady, L. (1995). *Curriculum Development*. Prentice Hall: Delhi. National Council of Educational Research and Training.
- Deng, Z. (2007). Knowing the subject matter of science curriculum, *Journal of Curriculum Studies*, 39(5), 503-535. https://doi.org/10.1080/00220270701305362
- Gronlund, N. E. & Linn, R. L. (2003). *Measurement and Assessment in teaching*. Singapore: Pearson Education
- McNeil, J. D. (1990). *Curriculum: A Comprehensive Introduction*, London: Scott, Foreman/Little
- Nehru, R. S. S. (2015). *Principles of Curriculum*. New Delhi: APH Publishing Corporation.
- Oliva, P. F. (2001). *Developing the curriculum* (Fifth Ed.). New York, NY: Longman
- Stein, J. and Graham, C. (2014). *Essentials for Blended Learning: A Standards-Based Guide*. New York, NY: Routledge.

Web Resources

- https://www.westernsydney.edu.au/ data/assets/pdf_file/0004/467095/Fundamentals_of_Blended_Learning.pdf
- https://www.uhd.edu/academics/university-college/centers-offices/teaching-learning-excellence/Pages/Principles-of-a-Flipped-Classroom.aspx
- http://leerwegdialoog.nl/wp-content/uploads/2018/06/180621-Article-The-Basic-Principles-of-Dialogue-by-Renate-van-der-Veen-and-Olga-Plokhooij.pdf