

CENTRAL UNIVERSITY OF PUNJAB



**Doctor of Philosophy
(Medicinal Chemistry)**

Batch – 2022

**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	L	T	P	Cr
1	CMC.701	Research Methodology & Biostatistics	4	0	0	4
2	CMC.702	Computer Applications	2	0	0	2
3	CMC.751	Research and Publication Ethics	2	0	0	2
4	CMC.752	Teaching Assistantship	0	0	2	1
5	UNI.753	Curriculum, Pedagogy and Evaluation	1	0	0	1
Opt for any one of the following courses						
7	CMC.705	Natural Products in Drug Discovery and Development: Recent Advances	4	0	0	4
8	CMC.706	Recent Advances in Medicinal Chemistry of Nucleic Acids	4	0	0	4
9	CMC.707	Emerging Trends in Green Synthesis and Drug Discovery	4	0	0	4
10	CMC.708	Trends in Molecular Modelling for Drug Design	4	0	0	4
		Total	13			14

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

Criteria of Evaluation:

End Term Examination: Subjective Type Test [100 Marks]

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

Course Contents

Unit/Hours	Content	Mapping with course learning outcomes
Unit 1 15 hours	<p>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.</p> <p>Intellectual Property Rights: Intellectual Property, intellectual property protection</p> <p>(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.</p> <p>Exercise: Design of research problem, data search, format, Components of IPR, Patent search/drafting</p>	CLO1, CLO2 and CLO3

<p>Unit 2 15 hours</p>	<p>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, Refworks, etc. Communication skills – defining communication; type of communication; techniques of communication, etc..</p> <p>Library: Classification systems, e-Library, Reference management, Web-based literature search engines</p> <p>Exercise: Drafting a manuscript, its reference management</p>	<p>CLO6</p>
<p>Unit 3 15 hours</p>	<p>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.</p> <p>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.</p> <p>Exercise: Numerical problems based on above-mentioned statistical techniques</p>	<p>CLO4</p>
<p>Unit 4 15 hours</p>	<p>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</p> <p>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.</p> <p>Exercise: Numerical problems based on above-mentioned statistical techniques</p>	<p>CLO5</p>

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**Paper Code: CMC.702****Learning Outcomes:**

L	T	P	Credits
2	0	0	2

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

CLO 1. Use and search various search engines for literature survey their research work.

CLO 2. Type, cite and edit the references of their thesis/dissertation work

Course Contents

Unit/Hours	Content	Mapping with course learning outcomes
Unit 1 8 hours	Fundamentals of computers: Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean algebra. Exercise: Problems based on Binary system, Logic gates and Boolean algebra.	CLO1
Unit 2 7 hours	MS Word (Word Processing, Creating and Saving Documents, Text Formatting, Tables, Document Review Option, Inserting Table of Contents), Powerpoint, Excel Sheet. Exercise: Draw a table using MS Word, Draw a ppt using Powerpoint and perform different functions on Excel Sheet.	CLO1
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. Exercise: Download an article using above-mentioned search engines	CLO1
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.	CLO2

	Exercise: Sketching of molecules using ChemBio Draw and reference management using EndNote	
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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/9780735669413.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 Title: Research and Publication Ethics

Paper Code: CMC.751

L	T	P	Credits
2	0	0	2

Learning outcomes of the course:

- Learners will be able to: -
- CLO 1. Define Ethics
- CLO 2. Interpret intellectual honesty and research integrity.
- CLO 3. List various open access publications
- CLO 4. Evaluate predatory publications and journals.

Course Contents

Unit/Hours	Content	Mapping with course learning outcomes
Unit 1 8 hours	<p>Philosophy and Ethics</p> <ul style="list-style-type: none"> • Introduction to Philosophy: definition, nature and scope, content, branches • Ethics: definition, moral philosophy, nature of moral judgements and reactions <p>Scientific Conduct</p> <ul style="list-style-type: none"> • 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 <p>Exercise: To make students aware about above-mentioned facts by using ppt</p>	CLO1 and CLO2
Unit 2 7 hours	<p>Applied Research in Media Studies</p> <ul style="list-style-type: none"> • 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 	CLO2 , CLO4

	<ul style="list-style-type: none"> • Violation of publication ethics, authorship and contributorship • Identification of publication misconduct, complaints and appeals • Predatory publishers and journals • Exercise: To make students aware about above-mentioned facts, Predatory publishers and journals by using ppt 	
Unit 3 8 hours	<p>Open Access Publishing</p> <ul style="list-style-type: none"> • 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. <p>Publication Misconduct</p> <ul style="list-style-type: none"> • 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 <p>Exercise: To arrange Group Discussions on Publication Misconduct and to check plagiarism by using above-mentioned resources</p>	CLO2 CLO3
Unit 4 7 hours	<p>Databases and Research Metrics</p> <ul style="list-style-type: none"> • 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 <p>Exercise: To h-index, g-index, i10 index of individual student/faculty</p>	CLO3

Suggested Readings:

1. Gregory, I. (2003). *Textbook of Research Ethics- Theory and Practice*. London: Bloomsbury Publishing PLC.
2. Oliver, P. (2003). *The student's guide to research ethics..* UK: Open University Press.
3. Shamoo, A.E., Resnik, D.B. (2015), *Responsible conduct of research*. USA: Oxford University Press.

4. Stanley, B.H., Sieber, J.B. Melton, G.B. (1996). *Research Ethics: A Psychological approach*. University of Nebraska.

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

Paper Code: CMC.705

L	T	P	Credits
4	0	0	4

Learning Outcomes:

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

CLO 1. Be familiar with the prospects of natural products

CLO 2. utilise the function of natural products in living organisms, their biosynthesis and medicinal properties in their practical

Course Contents

Unit/Hours	Content	Mapping with course learning outcomes
Unit 1 15 hours	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. Exercise: To discuss latest progress made in the field of natural/marine/herbal products	CLO1
Unit 2 15 hours	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. Exercise: To discuss latest progress made in the field of naturally occurring polyphenolic compounds	CLO1
Unit 3 15 hours	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	CLO2

	and Morphine, Recent developments in medicinal aspects- Antimicrobial activity, antioxidant and anti-inflammatory activities of alkaloids. Exercise: To discuss latest progress made in the field of alkaloids	
Unit 4 15 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. Steroids: determination and synthesis of cholesterol, Testosterone and Progesterone, Chemical tests for steroids, Medicinal applications of steroids. Exercise: To discuss latest progress made in the field of terpenoids	CLO2

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

Paper Code: CMC.706

Learning outcomes:

L	T	P	Credits
4	0	0	4

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

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

Course Contents

Unit/Hours	Content	Mapping with course learning outcomes
Unit 1 15 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. Exercise: To discuss latest progress made in the field of nucleic acids including conformation, size, shape, bending, supercoiling, post-transcriptional modifications and translations	CLO1
Unit 2 15 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). Exercise: To discuss latest progress made in the field of nucleic acids and understanding their interactions with drugs	CLO1
Unit 3 15 hours	Drug design and synthesis: Drugs targeting nucleic acids conformations, drugs targeting associated proteins, drugs mimicking, drugs targeting	CLO2

	<p>replication/transcription/translation and the proteins mentioned in unit 2. Drugs affecting gene expression (kinase inhibitors etc.)</p> <p>The SAR and <i>in silico</i> and pharmacokinetic approaches: to be discussed wherever possible in above-mentioned topics.</p> <p>Exercise: To discuss latest progress made in the field of nucleic acids using nucleic acids as drug targets</p>	
<p>Unit 4 15 hours</p>	<p>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.</p> <p>Exercise: To discuss role of SNPs small antisense RNAs (Si/micro RNA) in treatment of different diseases</p>	<p>CLO2</p>

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**

Paper Code: CMC.707

Learning outcomes:

L	T	P	Credits
4	0	0	4

After successfully completing this course learner would be able to:

CLO 1. Learn and draw the mechanism of microwave assisted organic transformation

CLO 2. Conduct ionic liquids, solid-supported organic reactions under MW and conventional conditions

CLO 3. Utilize metal and organocatalysts for various C-C and C-N bond formation reactions Apply recent tools in drug discovery and developments

Course Contents

Unit/Hours	Content	Mapping with course learning outcomes
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. Exercise: To perform microwave assisted synthesis	CLO1
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. Exercise: To perform microwave assisted synthesis using ionic liquid	CLO2
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 Exercise: To perform microwave assisted synthesis using metal catalysts	CLO3

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. Exercise: To perform microwave assisted synthesis of lead candidates/lead optimization using microwave assisted synthesis	CLO3
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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 α, 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 dihydrotageone 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:

L	T	P	Credits
4	0	0	4

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

CLO 1. How a slight change in substituents affect the biological activity of drugs?

CLO 2. How molecular modelling can increase efficiency.

CLO 3. Pharmacophore and receptor-based rational drug design.

Course Contents

Unit/Hours	Content	Mapping with course learning outcomes
Unit 1 15 hours	QSAR: Introduction, history, applications, various descriptors used in QSARs: lipophilicity, electronic, steric based descriptors. Regression analysis, significance and validity of QSAR regression equations, case study – on pyranamine, partial least squares (PLS) analysis, multi linear regression analysis. Use of genetic algorithms, neural networks and principle components analysis in the QSAR equations. Exercise: Solving problems related to multi linear regression, genetic algorithms, neural networks and principle components analysis	CLO1
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. Exercise: To perform 2D QSAR using free softwares	CLO2
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. Exercise: To perform 3D QSAR using free softwares	CLO3

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, <i>De novo</i> drug design. Exercise: To perform Virtual Screening and Molecular docking using free softwares	CLO3
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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. Lippincott 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

Course Code: CMC.752

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

CLO 1. familiarize themselves with the pedagogical practices of effective class room delivery and knowledge evaluation system

CLO2. 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.

Mapping with course learning outcome: CLO 1

- 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: UNI.753**Learning outcomes:****Total Hours: 15**

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

CLO 1. Analyze the principles and bases of curriculum design and development

CLO 2. Examine the processes involved in curriculum development

CLO 3. Develop the skills of adopting innovative pedagogies and conducting students' assessment

CLO 4. Develop curriculum of a specific course/programme

Course Content**Course Contents**

Unit/Hours	Content	Mapping with course learning outcomes
Unit 1 4 hours	Bases and Principles of Curriculum 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. Exercise: To understand Concept and Principles of curriculum	CLO1
Unit 2 4 hours	Curriculum Development 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. Exercise: Curriculum development according to NEP 2020	CLO2
Unit 3 3 hours	Curriculum and Pedagogy 1. Conceptual understanding of Pedagogy.	CLO3

	<p>2. Pedagogies: Peeragogy, Cybergogy and Heutagogy with special emphasis on Blended learning, Flipped learning, Dialogue, cooperative and collaborative learning</p> <p>3. Three e- techniques: Moodle, Edmodo, Google classroom</p> <p>Exercise: Using e- techniques: Moodle, Edmodo, Google classroom</p>	
Unit 4 4 hours	<p>Learners' Assessment</p> <p>1. Assessment Preparation: Concept, purpose, and principles of preparing objective and subjective questions.</p> <p>2. Conducting Assessment: Modes of conducting assessment – offline and online; use of ICT in conducting assessments.</p> <p>3. Evaluation: Formative and Summative assessments, Outcome based assessment, and scoring criteria.</p> <p>Exercise: Conducting quiz, group discussion</p>	CLO4

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>