# CENTRAL UNIVERSITY OF PUNJAB, BATHINDA



Doctor of Philosophy (Medicinal Chemistry)

Session – 2020 Course work

Department of Pharmaceutical Sciences and Natural Products

School of Basic and Applied Sciences

# **Program Outcome**

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 to start industry start up, great teacher and an independent scientist.



# **Course Structure**

# **SEMESTER 1 (Course Work)**

| S. No | Paper<br>Code | Course Title                                                              | L  | Т | P | Cr |
|-------|---------------|---------------------------------------------------------------------------|----|---|---|----|
| 1     | CMC.701       | Research Methodology                                                      | 4  | 0 | 0 | 4  |
| 2     | CMC.702       | Biostatistics                                                             | 2  | 0 | 0 | 2  |
| 3     | CMC.703       | Computer Applications                                                     | 2  | 0 | 0 | 2  |
| 4     | RPE           | Research and Publication Ethics                                           | 2  | 0 | 0 | 2  |
| *Opt  | any two of tl | he following courses                                                      |    |   |   |    |
| 5     | *CMC.704      | C.704 Natural Products in Drug Discovery and Development: Recent Advances |    |   |   | 3  |
| 6     | *CMC.705      | Recent Advances in Medicinal Chemistry of<br>Nucleic Acids                |    |   | 0 | 3  |
| 7     | *CMC.706      | Emerging Trends in Green Synthesis and Drug Discovery                     |    | 0 | 0 | 3  |
| 8     | *CMC.707      | Trends in Molecular Modelling for Drug Design                             |    | 0 | 0 | 3  |
| 9     | XXX.YYY#      |                                                                           | 3  | 0 | 0 | 3  |
|       |               | Total                                                                     | 16 |   |   | 16 |

<sup>\*\*</sup>Any other relevant course offered by faculty member of the same department or other department/School-To be decided by the respective supervisor.

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

Course Tile: Research Methodology

Paper Code: CMC.701 Learning Outcomes:

| L | Т | P | Credits |
|---|---|---|---------|
| 4 | 0 | 0 | 4       |

After successfully completing this course 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.

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.

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, Web-based literature search engines

Unit-3 15 hours

**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-4 15 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. (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.

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

**Course Tile: Biostatistics** 

| 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. Learn basic descriptive and inferential statistics including the concepts and principles of research design and statistical inference.
- 2. Perform and interpret descriptive and inferential statistical techniques including the Construction of tables and graphs, t-tests, Chi-square tests, and regression analysis.
- 3. Use appropriate software packages to solve analytical problems.

Unit 1 8 h

**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.

Unit 2 7 h

**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 3 7 h

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

Unit 4 8 h

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. Gookin, D. (2007). *MS Word for Dummies*. Hoboken, NJ: Wiley Publishing, Inc.
- 9. Harvey, G. (2007). MS Excel for Dummies. Hoboken, NJ: Wiley Publishing, Inc.
- 10. Sinha, P.K. Sinha, P. (2010). *Computer Fundamentals*. India: BPB Publications.
- 11. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials*. Canada: Decker Inc.
- 12. 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.
- 13. Bolton, S., & Bon, C. (2009). *Pharmaceutical statistics: practical and clinical applications*. Boca Raton: CRC Press.

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

Course Tile: Computer Applications

Paper Code: CMC.703

| L | T | P | Credits |
|---|---|---|---------|
| 2 | 0 | 0 | 2       |

## **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/sample pages/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.

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

Course Tile: Research and Publication Ethics

Paper Code: RPE

| L | T | P | Credits |
|---|---|---|---------|
| 2 | 0 | 0 | 2       |

## Learning outcomes of the course:

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

# 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: Applied Research in Media Studies

(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 contributorship
- 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

# 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 Tile: Natural Products in Drug Discovery

and Development: Recent Advances

| L | Т | P | Credits |
|---|---|---|---------|
| 3 | 0 | 0 | 3       |

# Paper Code: CMC.704 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 11 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 11 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 11 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 12 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.

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

Course Tile: Recent Advances in Medicinal

**Chemistry of Nucleic Acids** 

| L | Т | P | Credits |
|---|---|---|---------|
| 3 | 0 | 0 | 3       |

Paper Code: CMC.705

## 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 11 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 11 h

**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 11 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 above mentioned topics.

Unit 4 12 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.

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

Course Tile: Emerging Trends in Green
Synthesis and Drug Discovery

Paper Code: CMC.706

| L | T | P | Credits |
|---|---|---|---------|
| 3 | 0 | 0 | 3       |

## Learning outcomes:

After successfully completing this course learner would be able to:

- 1. Learn and draw 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 11 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 11 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 11 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 12 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.

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

Course Title: Trends in Molecular Modelling for

**Drug Design** 

Paper Code: CMC.707

| L | т | P | Credits |
|---|---|---|---------|
| 3 | 0 | 0 | 3       |

## Learning outcomes:

After successfully completing this course learner would be able to:

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

Unit 1 12 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 11 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 11 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 11 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.

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