NIRMA UNIVERSITY
Institute of Pharmacy
(B. Pharm)
(Semester - VIII)

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Course Code	**BP807ET**
Course Title	**Computer Aided Drug Design - Theory**

Scope:
This subject is designed to provide detailed knowledge of rational drug design process and various techniques used in rational drug design process.

Objective: Upon completion of the course, the student shall be able to understand -

1. Design and discovery of lead molecules.
2. The role of drug design in drug discovery process.
3. The concept of QSAR and docking.
4. Various strategies to develop new drug like molecules.
5. The design of new drug molecules using molecular modeling software.

Course Learning Outcomes (CLO):
After successful completion of the course, student will be able to –

1. Understand the role of molecular mechanics and quantum mechanics in molecular modeling.
2. Describe various stages of lead design, drug discovery and development process.
3. Discuss concepts and applications of different molecular modeling techniques.
4. Explain the role of quantitative structure-activity relationship (QSAR) studies in rational drug design.
5. Use various informatics and methods in drug design.

Syllabus: **Teaching hours: 45 Hours**
Study of the development of the following classes of drugs, Classification, mechanism of action, uses of drugs mentioned in the course, Structure activity relationship of selective class of drugs as specified in the course and synthesis of drugs superscripted (*).

UNIT I **10 Hours**

Introduction to Drug Discovery and Development

- Stages of drug discovery and development

Lead discovery and Analog Based Drug Design

- Rational approaches to lead discovery based on traditional medicine, Random screening, Non-random screening, serendipitous drug discovery, lead discovery based on drug metabolism, lead discovery based on clinical observation.

Analog Based Drug Design

- Bioisosterism, Classification, Bioisosteric replacement. Any three case studies.

UNIT II **10 Hours**

Quantitative Structure Activity Relationship (QSAR)

- SAR versus QSAR, History and development of QSAR, Types of physicochemical parameters, experimental and theoretical approaches for the determination of physicochemical parameters such as Partition coefficient, Hammet's substituent constant and Tafts steric constant. Hansch analysis, Free Wilson analysis, 3D-QSAR approaches like COMFA and COMSIA.

UNIT III **10 Hours**

Molecular Modeling and virtual screening techniques

Virtual Screening techniques

- 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

UNIT IV **08 Hours**

Informatics & Methods in drug design

- Introduction to Bioinformatics, chemoinformatics. ADME databases, chemical, biochemical and pharmaceutical databases

UNIT V **07 Hours**

Molecular Modeling

- Introduction to molecular mechanics and quantum mechanics. Energy Minimization methods and Conformational Analysis, global conformational minima determination.

Tutorials **15 Hours**

Tutorials will be based on above syllabus.

Suggested Readings^: (Latest edition)

1. Robert, G.C.K. ed. *Drug Action at the Molecular Level*. University Prak Press Baltimore.
2. Martin, Y. C. (2010). *Quantitative drug design: a critical introduction*. CRC Press.
3. Wilson, C. O., Beale, J. M., & Block, J. H. Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry. Lippincott Williams & Wilkins.
4. Foye, W. O. Foye's principles of medicinal chemistry. Lippincott Williams & Wilkins..
5. Koro l.A. Burckhalter J.H. *Essentials of Medicinal* Chemistry. Wiley Interscience
6. Burger, A., & Abraham, D. J. *Burger's medicinal chemistry and drug discovery* (Vol. I–IV). Wiley.
7. Patrick, G. L. (2013). *An introduction to medicinal chemistry*. Oxford university press.
8. Smith, H. J., & Williams, H. (2016). *Introduction to the principles of drug design*. Elsevier.
9. Silverman, R. B., & Holladay, M. W. (2014). *The organic chemistry of drug design and drug action*. Academic press.

L= Lecture, T= Tutorial, P= Practical, C= Credit

^ This is not an exhaustive list