ICS 505: COMPUTER AIDED DRUG DESIGN

The subject is designed to impart knowledge on the current state of the art techniques involved in computer assisted drug design

Objectives: Upon completion of this course the student should be able to

- Role of CADD in drug discovery
- Different CADD techniques and their applications
- Various strategies to design and develop new drug like molecules
- Working with molecular modeling softwares to design new drug molecules
- The *in silico* virtual screening protocols

UNIT I **12hr**

Introduction to Computer Aided Drug Design (CADD) History, different technique sand applications Quantitative Structure Activity Relationships: Basics History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters (sigma), lipophilicity effects and parameters (log P, pi substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physicochemical parameters Quantitative Structure Activity Relationships Deriving 2D-QSAR equations 3D-QSAR approaches and contour map analysis Statistical methods used in QSAR analysis and importance of statistical parameters

UNIT II **12 hr**

Molecular Modeling and Docking A) Molecular and Quantum Mechanics in drug design B) Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation C) Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra-precision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AchE & BchE) Molecular Properties and Drug Design: a) Prediction and analysis of ADMET properties of new molecules and its importance in drug design. b) De novo drug design: Receptor/enzyme-interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design. c) Homology modeling and generation of 3D-structure of protein

UNIT III **10hr**

Pharmacophore Mapping and Virtual Screening Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modeling; Conformational search used in pharmacophore mapping In Silico Drug Design and Virtual Screening Techniques Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols 12

REFERENCES:

1. Computational and structural approaches to drug discovery, Robert M StroudandJanet.F Moore,RCS Publishers.
2. Introduction to Quantitative Drug Design by Y.C. Martin, CRC Press, Taylor&Francis group..
3. Drug Design by Ariens Volume 1 to 10, Academic Press, 1975, Elsevier Publishers.
4. Principles of Drug Design by Smith and Williams, CRC Press, Taylor & Francis.
5. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, Elsevier Publishers.
6. Medicinal Chemistry by Burger, Wiley Publishing Co
7. An Introduction to Medicinal Chemistry –Graham L. Patrick, Oxford University Press.
8. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ippincott Williams & Wilkins.
9. Comprehensive Medicinal Chemistry – Corwin and Hansch, Pergamon Publishers.
10. Computational and structural approaches to drug design edited by Robert M Stroudand Janet. F Moore