Mar Thoma College Chungathara
Department of Chemistry
Syllabus on Drug design and Machine learning

UNIT I

Introduction to Cheminformatics & Drug Discovery

Cheminformatics; Introduction, history of cheminformatics, scope of cheminformatics, learning in cheminformatics, data; data, information, knowledge, representation and manipulation of 2D and 3D molecular structures, Chemical file formats; mol files, SDFiles, inter conversion of file formats, markush structures, molecular surfaces; vander waals surface, connolly surface, solvent-accessible surface, solvent excluded surface, visualization of molecular models; wire frame model, capped sticks model, ball and sticks model, space filled models, chemical spaces.

UNIT II

Introduction to Chemical and Biological databases

Chemical databases; pubchem database, pubmed database, zinc database, e-molecules database, Chemspider, PDB, UNIPROT, etc.

UNIT II

Structure based and Ligand-Based Drug Design

Introduction to Structure based drug design; Ligand, Target, Docking, Introduction to Ligand-based drug design, application, Absorption, Distribution, Metabolism, Excretion & Toxicology (ADMET) prediction.

References

1. *Chemoinformatics in Drug Discovery, Tudor I. Oprea (Editor), Raimund Mannhold (Series Editor), Hugo Kubinyi (Series Editor), Gerd Folkers (Series Editor),* Wiley-Vch Publishers, NY (2005).
2. *Chemoinformatics: A Textbook*, Johann Gasteiger (Editor), Thomas Engel (Editor), Wiley-Vch Publishers, NY (2003).
3. *An Introduction to Chemoinformatics*, Andrew R. Leach & Valerie J. Gillet, Kluwer Academic Publishers, Boston, MA (2003).

4. "*An Introduction to Medicinal Chemistry*" fourth edition, Graham L., Patrick.