IT- 762 : Chemoinformaties In drug designing (Chemoinformatics) (3 credits)

Prerequisite:. Courses on Structural Bioinformatics, Basic Biochemistry/Chemistry and Perl/Python

Objectives

In the present drug industry is starving for a trained informatics having a good knowledge in Computational biology, mathematics, statistics, chemistry, pharmacology & computer language. The course M.tech at SIT provides a well trained student with basic knowledge in computer language, mathematics, statistics and computational biology, this additional optional course offers those students who would like to acquire enough knowledge for the above mentioned skills and to orient themselves in the field of drug designing industry. Orientation of this course is to provide a hands-on experience in the challenging field of post-genomic drug discovery.

Syllabus: (10 hrs)

Logic of designing chemicals
Chemical information systems
In silico generation of virtual molecules
Structure Search, Similarity and Property Estimation
Pharmacophore modeling and lead identification
Lead Optimization and Library Design

Target Identification, Prioritization and Validation (5 hrs)
Comparative proteomics/Genomics: Protein annotation and function assignment.
Mining Gene Expression Data, Biochemical Pathway Analysis & Mechanism of action
In silico Structure based drug discovery

ADMET and PK/PD: Hit to Lead to Drug (5 hrs)
Prediction of Absorption and Molecular Physical Properties
Permeability/Solubility/Stability(LogP/LogD/pKa)
Models for P450-mediated Metabolism
Modeling/prediction of Toxicity
Pharmacokinetics/Pharmacodynamics: *in silica* modeling and estimation of parameters

Case Studies: Viral System(H1V / Dengue viruses) (5 hrs)
Cardiovascular/Inflammatory/Cancer (5)
Practical/Assignment (15)

Propose and Design any one of the followings :
Disease Specific Chemical Designing
Target specific inhibitor designing
Ligand Based inhibitor Designing
QSAR/QSPR

Suggested readings:

Juan Alvarez and Brain Shoichet, Virtual Screening in Drug Discovery; Edited by Tudor I. Oprea, Chemoinformatics in Drug Discovery;
R.E. Babien and S.S. Adbel-Meguid, Protein Crystallography in Drug Discovery; Johann Gasteiger and Thomas Engel, Chemioinformatiics ;
Susanna Wu-Pong, PhD Yon Rojanasakul , Han Van de Waterbeemd, Structure-Property correlations in Drug Research ;

Hugo Kubinyi, Gerd Folkers and Yvonne C. 3D Qsar in Drug Design Ligand Protein Interactions and Molecular Similarity Volume 2. In Biopharmaceutical Drug Design and Development Second

Edition:
Rajesh Krishna Lawrence Yu Editors, Biopharmaceutics Applications in Drug Development ; Frank Petersen Rene Amstutz Editors,Natural Compounds as Drugs, Volume I & Vol II; M.Hamacher, K. Marcus, K. Stuhler, Proteomics in Drug Research;
James M.Brower, Hamid Bolouri, Computational Modeling of Genetic and Biochemical Networks; C.Stan Tsai, Computational Biochemistry ;
Aidong Zhang, Advanced Analysis of Gene Expression Microarray Data;
Isaac S. Kohane, Alvin T. Kho, And Atul J. B., Microarrays for an Integrative Genomics; Dov Stekel, Microarray Bioinformatics.