Bioinformatics and Computer Aided Drug Designing

Syllabus

Theory

Module I 5 hrs

Introduction to Bioinformatics, Biological Databases: Biological Sequence Databases - NCBI, EMBL, DDBJ, PIR, SWISS-PROT; Protein 3D Structure and Classification Databases - PDB, MMDB, CATH, SCOP

Module II 4 hrs

Basic idea of sequence comparison- Pair wise and multiple sequence alignment. Sequence analysis software's- BLAST, FASTA, CLUSTAL.

Module III 4 hrs

Protein structure prediction, Homology modelling - Swiss-model, *ab initio* modelling, Molecular Visualization Software's - SWISS-PDB Viewer

Module IV 5 hrs

Drug Designing, Molecular Docking, Auto Dock, Discovery Studio.

Practicals

12 hrs

1. Familiarizing with the different data bank mentioned in the syllabus.

2. Retrieve a document reporting recent work on a genomic analysis of human disease.

3. Retrieve one sequence both DNA and protein from database retrieval systems.

4. Familiarizing with sequence analysis tools - BLAST, FASTA and CLUSTAL

5. Molecular Visualization with Swiss-PDB Viewer.

6. Molecular docking with Auto Dock.

7. Hands on training in commercial bio-software Discovery Studio.