

TRAINING CONTENT:

Introduction to biological databases

Introduction to genomics, Gene prediction methods and tools. Basic structures of nucleotides
Introduction to biological databases - primary, secondary and composite databases, Data storage and formats.

NCBI, Nucleic acid databases (GenBank, EMBL, DDBJ), protein databases (PIR, Swiss-Prot, TrEMBL, PDB), Metabolic pathway database – KEGG.

Small molecule databases (PubChem, Drug Bank, ZINC).

Protein domains, conserved domains and repeats analysis.

Sequence alignment and Phylogenetic analysis

Alignment – local and global alignment, pair-wise and multiple sequence alignments.

Alignment algorithms, BLAST and CLUSTALW, Amino acid substitution matrices (PAM and BLOSUM). Multiple sequence alignments, Construction of phylogenetic tree and dendrograms.

Protein structure prediction

Amino acid structures, Levels of protein organization – Primary, Secondary, Tertiary & Quaternary structures. Protein secondary structure prediction, 3D structure building using homology modeling, Ramachandran Plot.

Molecular docking

Protein preparation, Ligand preparation, Grid generation, docking algorithms, Docking analysis, virtual screening.

Introduction to molecular dynamics (theory class on Gromacs)