

Course: Bioinformatics  
Teacher: Gianluca Molla  
Length: 2.5 CFU (20 hours)

Objective:

Provide student with practical knowledge of the main bioinformatic processes used in protein investigation. All lessons will be held at the computer, in an informatics class. Most of procedures shown will be performed by the students themselves under the supervision of the teacher. Results will be discussed in a critical manner.

COURSE TOPICS

The course will cover the main topics of the bioinformatics approach to the study of the structure/properties of the proteins. In details:

1. The format of structural data and structural databases (PDB files, RCSB, PDBeChem, ...) and how to search and retrieve structural information
2. Basis of visualization of 3D structures and software for macromolecule visualization (PyMol, VMD, ...)
3. Prediction of structural properties of proteins (secondary structure, transmembrane regions, signal peptides, ...)
8. Discover the evolutionary history of a protein: build a phylogenetic tree, detect the most conserved positions and predict the sequence of ancestral proteins
4. Construction of models of the 3D structure of a protein (*ab initio* modelling, homology modelling)
5. Build models of variants *in vitro* - foldX - ProSAR
6. Prediction of binding of small ligands (e.g., drugs) to proteins by Automated Molecular Docking
7. Prediction of quaternary structure haddock, Z-DOCK
8. Simulation of protein flexibility in solution: The Molecular Dynamics approach