Laboratory of Bioinformatics 1

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- X-ray diffraction gives us diffracrtion maps
- Diffraction maps are interpreted by Fourier transform to compute the electron density
  - It is a computation-heavy task
- Electron density is used to fit a protein structure
- I compute the diffraction pattern of the theoretical protein structure to check if it matches the experimental pattern within a reasonable tollerance
- The PDB file does not contain the electron density, it is an approximation of the structure
- The only textbook is PDB-101
- The resolution of an X-ray diffraction is imprtant
  - 5.0Å resolution is reasonably accurate only for the position of the backbone
  - 1.5Å can be generally trusted, also for drug design
- We need to know the Bragg diffraction law
- Crio-electron microscopy gives us a diffraction pattern using an electron beam
  - It is really useful for really big complexes that cannot be cristallized
  - Resolution is lower than X-ray diffraction
- A ligand is any molecule co-cristallized with the macromolecule considered
- Biology without structure is fantasy
- Annotation is an inference where you endow with structural and functional features an element
- A PDB file has an unique identifier of 4 letters and numbers
- On PDB I can also find the FASTA of the protein
  - FASTA contains the covalent structure (i.e the sequence) of the protein
  - It is the sequence derived from the structure, it can be different than the one in uniprot (!)
- Signal peptides are 10 to 30 residues in length
  - They are usually cleaved and therefore they do not appear in the protein 3d strucutre
- Coverage refers to the percentage of protein sequences covered in the protein structure
- FASTA has 60 residues per line
- Routinely X-ray diffraction is not able to locate hydrogens
- Each crystal has a unit cell
- PDB files produced using a synchrotron source have 2 spots associated with every atom
- For each ATOM we have the xyz coordinates, the occupancy, and temperature factor
  - Occupancy is how well the atom fits the electron density
  - The temperature factor refers to the mobility of the position
- The PDB file contains the atomic model of a macromolecule
- The CPK colorscheme is a popular set of colors used for the different atoms
- The structure validation window reports the percentile rank of different validation methods
  - Blue is good, red is bad
- DSSP is a program that reads a PDB file and assigns a secondary structure to each PDB coordinate
  - It was made by Sanders, one of the founders of bioinformatics, and Kabsch