**Curso de Diseño de Fármacos**

**Visualización molecular**

1. **Retrieval of** PDB **Files**. Using the web PDB browser, find coordinate files for the crystal forms II and III of Bovine Pancreatic Trypsin Inhibitor (BPTI) among the many BPTI entries. Notice that one has exceptionally the corresponding hydrogens.
2. **Format of** PDB **Files**. Read the text in the top of both PDB files and describe the differences in the number of recorded residues, structure resolution, number of solvent molecules, experimental conditions, etc. Attach to the assignment sheet a printout of a few lines, starting with the word ATOM, from a PDB file; mark with arrows and describe the content of each specific format field. (The PDB browser contains information about the format; see also the original paper on PDB files: *J. Mol. Biol.* **112**, 535–542, 1977).
3. **Protein Retrieval and Visualization of Myoglobin**
   1. Use the Protein Data Bank (PDB) to find Myoglobin.
   2. Explain where the data that gets deposited in the Protein Data Bank come from.
   3. Obtain the primary amino acid sequence of Myoglobin (FASTA) via PDB.
   4. Determine how many amino acids are in myoglobin, how many histidines are present, and at what positions.
   5. Which amino acids are at the N and C terminus; which amino acid is the first in the myoglobin protein chain?
   6. Identify the secondary structure of Myoblobin.
   7. Find the Histidines in Myoglobin that make close contact with the Heme small molecule.
4. **Bovine Pancreatic Trypsin Inhibitor**:
   1. Retrieve from PDB the file of mutated form C30A/C51A of BPTI (7pti).
      1. Superimpose all BPTI proteins.
      2. Label residues in one of them (all and part of the protein).
      3. Inspect disulfide bonds in all of them.
      4. In few paragraphs describe the structural differences between both forms of BPTI.
      5. Observe occupancy in R42 in all three structures.
   2. Conversion: Delete all hydrogens and convert from x-ray to ICM object (use of “convert”).
   3. Ramachandran Plots.
      1. Let’s study first how to extract information from ICM. Perform “ds a\_/32,33,34 only” on a converted structure.
      2. Identify the *ϕ* and *ψ* angles of each residue using v\_/xxx/psi,phi
      3. Collect angles in an array and export.
      4. Collect angles in a table and export.
      5. Build Ramachandran plot.