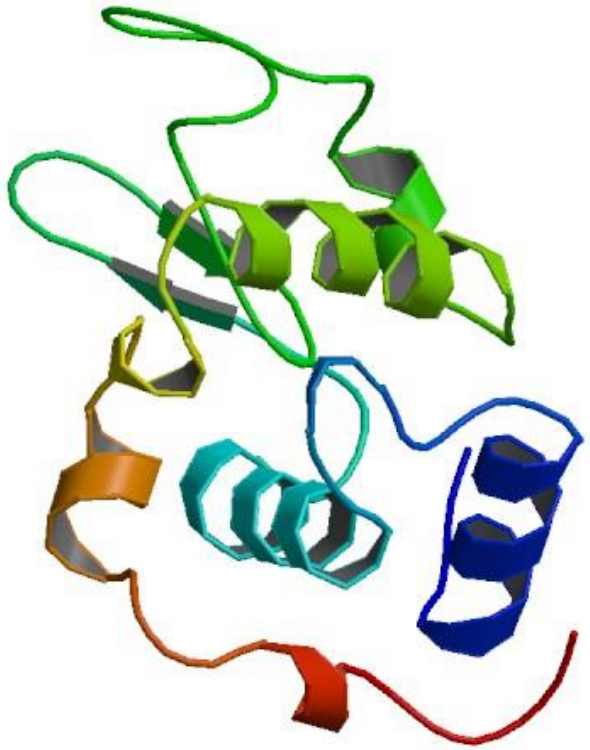
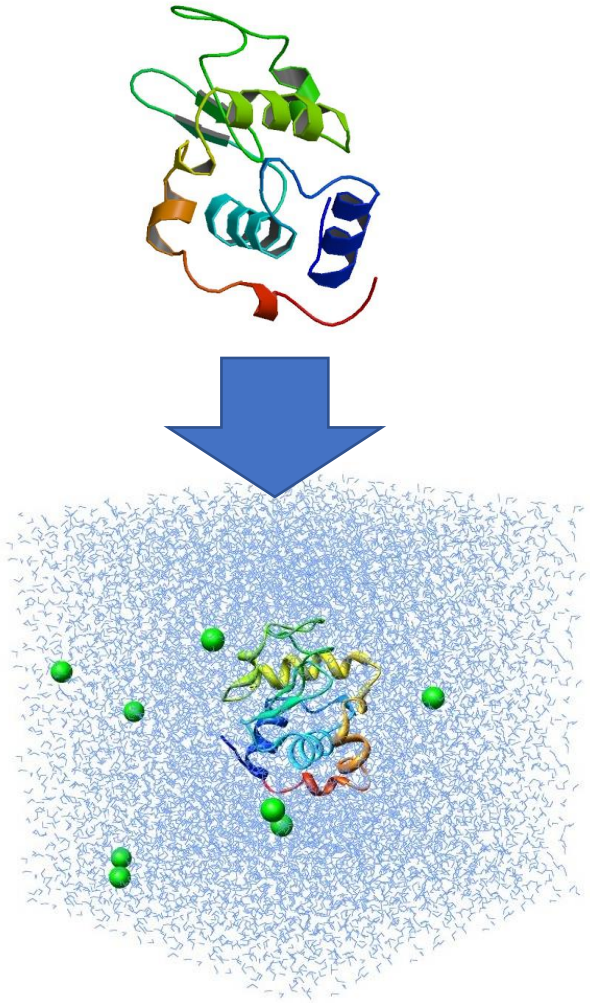
Content of the 1st exercise



- How to find crystal structures of proteins
- Setting up and run a molecular modelling simulation of a small protein
- Analyze the simulation data

How to do a molecular dynamics simulations study for a practical biomolecular system (the small protein)



- Research question?
  - Modelling method according to the relevant length and time scales involved in the phenomena.
  - Design molecule study system so that matches the research question.
  - Appropriate environment (in atomistic detail modelling, for example, solvent such as water and ions or added salt)
- Simulation needs defined
  - “size” -> simulation box
  - “boundaries”
  - Interactions of all atoms / molecules in the system (force-field)
  - Choice of statistical mechanics ensemble (Gibbs free energy / isothermal-isobaric ensemble most common for chemical and biomolecular systems). *T* and *p* controlled by algorithms.
  - System conditions such as molecular concentrations, pressure *p*, temperature *T*, …
  - How is time evolution obtained? Integration algorithm for the equations of motion resulting from forces on each particle.
- Analysis methods / analysis questions

A GROMACS workflow for exercise 1. The workflow takes a PDB (Protein Data Bank) structure file as input and returns a MD trajectory.