

Questions for the mid-term evaluation
Panel: advanced structural methods

Part 1: Crystallography 1

1. Phasing problem in crystallography, Patterson method and direct methods.
2. Direct space methods in structure solution. Simulated annealing methods.
3. Direct space methods in structure solution. Grid search method, pros and cons.
4. Charge flipping method in structural analysis.
5. Powder diffraction methods in materials chemistry.
6. Full profile approach – Rietveld method. Differences between powder XRD and single crystal XRD.

Part 2: Crystallography 2

1. PDB and CSD – what types of molecular structures can be found in these databases and what types of structural information can be collected during analysis of data deposited there?
2. Explain the importance of resolution, R factors and electron density interpretation on the structural data reliability of biological macromolecules for their potential use in molecular docking procedures.
3. Describe basics of particular docking procedures:
 - a) rigid body
 - b) semi-elastic
 - c) elastic
4. What is the scoring function and how its value can be used to interpret docking results (based on PLP function of Gold program).
5. What types of non-covalent interactions can stabilize a ligand-protein complex?