Part 1

Computational

1. Discuss the application of triangular decompositions of matrices to solve the systems of linear equations.
2. Discuss the application of similarity transformations to solve the eigenproblem of a matrix.
3. Discuss the use of matrix pseudoinverse to find the minimum solution of a system of linear equations.
4. Give and discuss briefly examples of a single-step and a multi-step method used to integrate ordinary differential equations.
5. Compare two classes of methods used in optimization: gradient-based and not evaluating gradients.

Part 2:

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 3:

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?