Self-assessment quiz for young scientist interested in autumn school "Biomolecular Structure and Function – Computational Approaches"

These questions are intended for self-assessment of your state of knowledge. If you intend to participate in the autumn school, you should be able to answer seven or more of these questions comfortably in less than an hour. This includes the time for Google, web searches and looking things up in the textbooks you used during your studies. As a scientist, you should be honest to yourself, as always, but also because the autumn school will just be a waste of your time and no fun at all if you lack the basic knowledge that is underlying these questions.

1. Thought experiment: You put living organisms with food into a large box so that it is completely isolated from its environment (no exchange of heat or substance). What will happen to the organisms if you wait for a long time? Can you argue with a physical law? If yes: with which law?

2. You have a sodium ion and a chloride ion at a distance of 1 nm, (a) in vacuum, (b) in water. Estimate the ratio of potential energies between the two cases, with the potential energy at infinite distance set to zero.

3. Why do Heparin-binding proteins often have many basic groups?

4. Why are ionic amino acid residues rarely found inside proteins, but frequently on the surface?

5. Flexible ligands often bind with lower affinity to proteins compared to similarly composed but more rigid ligands. What could be the reason for this?

6. Is the following sequence more likely to form an amphiphilic helix or a beta strand: **IENVAKKILQDK**? Explain your choice!

7. The sequence in question 6. has been taken from a real protein for which an experimental X-ray structure exists. From which protein?

8. You have the amino acid sequences of two large proteins A and B. Someone claims: A and B are totally different except for one domain, for which homologous domains are present in A and B. By which standard method could this claim be tested easily?

9. How many residues does a protein of 5000 non-hydrogen atoms roughly have? Can you sketch pseudo code for a program that calculates the radius of the protein (assumed to be spherical) given that you have, of course, the (x,y,z) coordinates of all atoms?

10. Person 1 says, she has found experimentally that the 3D-structure of protein X is a beta barrel, while person 2 claims that X has a purely helical structure. Can you settle the dispute by computational modelling? If yes: how? If no: why not?