BioPhysics - BIO361
Quiz2
30.11.24

Total marks :20
Time : 1hr

MCQ(1*10=10 marks)

1. Which file format in MD simulations is updated after each step during the simulation to store the evolving atomic positions and velocities?
   a) .pdb
   b) .trr
   c) .top
   d) .mdp

2. What is the primary purpose of energy minimization in MD simulations?
   a) To equilibrate the system to a desired temperature
   b) To remove steric clashes and unrealistic forces in the system
   c) To calculate the free energy of the system
   d) To set up periodic boundary conditions

3. Which of the following best describes the role of the force field in MD simulations?
   a) Defines the boundary conditions for the simulation box
   b) Determines the integration step size for time evolution
   c) Provides mathematical equations and parameters for interatomic interactions
   d) Simulates quantum mechanical effects on atoms

4. In MD simulations, why is the time step critical to the accuracy and stability of the simulation?
   a) Larger time steps increase the resolution of the trajectory.
   b) Time steps are irrelevant to energy conservation.
   c) A time step must be small enough to capture atomic vibrations accurately.
   d) Smaller time steps decrease computational cost.

5. Which of the following file formats in MD simulations specifies the molecular interactions, including atom types, bonds, and parameters for the system?
   a) .gro
   b) .pdb
   c) .top
   d) .mdp

6. What is the purpose of the `.ali` file in Modeller?

a) To specify the force field used in modeling

b) To define the sequence alignment between the target and the template(s)

c) To store the output structure of the modeled protein

d) To provide visualization parameters for the model

7. In single-template modeling with Modeller, what is the primary factor that determines the accuracy of the final model?

   a) The resolution of the template structure

   b) The energy minimization parameters used

   c) The number of templates used

   d) The size of the simulation box

8. How does Modeller handle regions of the target sequence that are not covered by any template?

   a) It leaves those regions undefined.

   b) It uses loop modeling to predict the structure of those regions.

   c) It excludes those regions from the final model.

   d) It forces the structure to match the nearest template region.

9. In advanced multi-template modeling, what method does Modeller use to incorporate multiple templates into a single model?

   a) By taking a direct average of all template coordinates

   b) By weighting contributions based on alignment quality and sequence identity

   c) By selecting one template at random for each region

   d) By manually selecting which template to use for each residue

10. What is the main advantage of using multiple templates in Modeller over a single template?

    a) It reduces the computational time for building the model.

    b) It allows structural diversity to improve model accuracy and coverage.

    c) It ensures that all templates have the same resolution.

d) It eliminates the need for sequence alignment.

Short answer type questions (2 * 5=10 marks)

1. In multi-template modeling, what is the primary file format used to provide the structural templates to Modeller? What command in Modeller is used to align the target sequence with template structures?

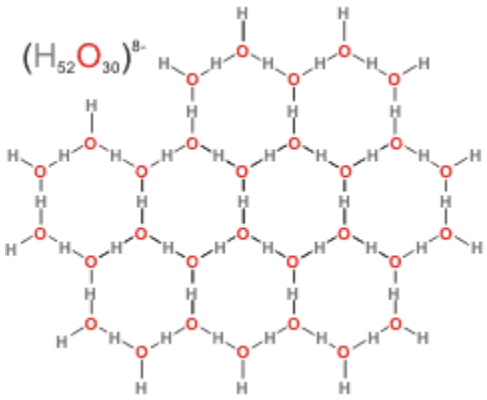
   The primary file format used to provide the structural templates to Modeller is **PDB (Protein Data Bank format)**. The command used in Modeller to align the target sequence with template structures is `salign`.

2. How does poor alignment between the selected template and the query sequence, or the improper selection of multiple templates, impact the quality of the generated model in Modeller?

   Poor alignment or improper selection of templates can significantly reduce the quality of the generated model. If the alignment is incorrect, structural information from the template is transferred inaccurately to the model, leading to errors such as incorrect folding, misaligned secondary structures, or unrealistic geometry. Similarly, conflicting information from improperly selected multiple templates can cause structural artifacts, reducing the reliability of the model. Proper alignment and template selection are crucial to ensure that the structural features of the model are accurate and biologically relevant.

3. Explain why "Polywater," initially thought to be a polymerized form of water, was later dismissed as a scientific misconception. Make a diagram as well.

   "Polywater" was initially believed to be a novel form of water with unusual properties like higher viscosity and density. However, further investigations revealed that these properties were due to contamination from impurities such as sweat, oils, or experimental apparatus residues, rather than a new polymerized form of water. Advances in analytical techniques and better experimental controls disproved the existence of polywater, showing that it was an artifact of experimental contamination.



4. How does volume, or microstates complicate the boltzmann distribution

   Volume and microstates complicate the Boltzmann distribution because they directly affect the entropy and energy levels of the system. The Boltzmann distribution predicts the probability of a system occupying a particular energy state based on the number of accessible microstates. Larger volumes increase the number

of microstates, which in turn increases the entropy. This requires complex integrations over all possible states, making the computation of probabilities and partition functions more difficult. Moreover, as the number of microstates increases, distinguishing between individual contributions to the overall distribution becomes challenging.

5. What is the hydrophobic effect, and which types of interactions are responsible for it?

   The **hydrophobic effect** is a fundamental phenomenon that describes the tendency of nonpolar molecules or molecular regions to aggregate in an aqueous environment. This behavior minimizes the unfavorable interactions between nonpolar substances and water while maximizing favorable water-water interactions. The hydrophobic effect is crucial for many biological processes, including protein folding, membrane formation, and molecular recognition.

   Water-Water Hydrogen Bonding:

   Water molecules maintain their hydrogen bond network by rearranging around nonpolar surfaces, leading to the hydrophobic effect.

   Dispersion Forces (Van der Waals):

   Once nonpolar molecules aggregate, weak dispersion forces between them contribute to their stabilization.