Session 2 Quiz

**1. What is the purpose of energy minimisation?**

a) Increase the system’s temperature

b) Minimise the forces and potential energy

c) Increase the kinetic energy

d) Adjust the simulation box size

**2. In the context of molecular dynamics, what does NVT stand for?**

a) Constant number of particles, volume and temperature

b) Normalized Velocity Trajectory

c) Constant number of molecules, velocity and temperature

d) constant number, volume and trajectory

**3. In protein simulations, which particles are typically restrained during equilibration?**

a) Hydrogen atoms

b) Water molecules

c) Protein heavy atoms

d) Ions

**4. Which command adds ions to the solvated protein system in GROMACS?**

a) gmx ions

b) gmx add-ions

c) gmx genion

d) gmx charge

**5. What information can be gained from the root-mean-square deviation (RMSD) in protein simulations?**

a) Changes in system temperature between the start and the end of the simulation

b) Changes in the protein structure over simulation time

c) Solvent interactions with a folded protein

d) The electrical charge distribution within the protein

**6. What type of boundary conditions are typically used in molecular dynamics simulations to mimic an infinite system?**

a) Reflective boundary conditions

b) Periodic boundary conditions

c) None, boundaries are not defined

d) Open boundary conditions

**7. What does the emtol parameter in the .mdp file specify?**

a) The temperature of the system

b) The energy tolerance value

c) The number of atoms

d) The simulation time step

**8. Which command prepares the .tpr input file for a GROMACS simulation?**

a) gmx solvate

b) gmx mdrun

c) gmx editconf

d) gmx grompp

**9. What command is used to calculate how the temperature changes during a**

**simulation?**

a) gmx temp

b) gmx energy

c) gmx calculate

d) gmx solvate

**10. Which of the following quantities can be modelled with the aid of molecular dynamics simulation?**

a) Density of molecular system under given conditions

b) Colour changes in chemical reactions

c) Electronic structure of a photochemically excited molecule

d) All of the above