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. Which algorithm is typically used for energy minimisation in GROMACS?**

a) Genetic algorithm

b) Simulated annealing

c) Steepest descent

d) Newton's method

**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

b) Structural stability over time

c) Solvent interactions

d) Force field accuracy

**6. What does the radius of gyration indicate in a protein simulation?**

a) Energy minimization efficiency

b) Protein compactness and folding state

c) Solvent density

d) Simulation duration

**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 is the main aim of the NPT equilibration phase?**

a) Set temperature to 0 K

b) Equilibrate density and pressure

c) Maximize energy

d) Remove solvent molecules

**10. What command is used to calculate how the temperature changes during a simulation?**

a) gmx energy

b) gmx temp

c) gmx calculate

d) gmx solvate