Session 2 Pre-Quiz

**1. Which of the following must be run before a simulation can be run to collect data?**

a) Energy minimisation

b) NVT equilibration

c) NPT equilibration

d) All of the above.

**2. During which phase is the system stabilised at a constant temperature?**

**a) Energy minimization**

**b) NPT equilibration**

**c) NVT equilibration**

**d) Production run**

**3. Which command allows you to view the last 10 lines of a file?**

a) head -l 10

b) tail -n 10

c) more -l 10

d) cat -n 10

**4. Why is it important to check potential energy during energy minimisation?**

a) To validate the force field

b) To ensure stable molecular structure

c) To optimize pressure

d) To adjust box size

**5. Why is solvation important in protein simulations?**

a) It increases computational power

b) It mimics the protein’s natural environment

c) It stiffens the protein structure

d) It reduces molecular dynamics

**6. Which software is frequently used for visualizing molecular dynamics trajectories?**

a) Photoshop

b) VMD

c) Excel

d) AutoCAD

**7. What is the purpose of using a thermostat in protein simulations?**

a) To change the colour scheme

b) To apply harmonic restraints

c) To control system temperature

d) To remove periodic boundaries

**8. What components are typically included in molecular mechanics force fields?**

a) Bond lengths, angles, and torsions

b) Atom colours and sizes

c) Simulation speed and duration

d) Protein sequence and structure

**9. Which GROMACS command would you use to calculate pressure changes?**

a) gmx calculate

b) gmx energy

c) gmx editconf

d) gmx pressure

**10. Which command solvates the protein in GROMACS?**

a) gmx insert-molecules

b) gmx solvate

c) gmx add-ion

d) gmx build