Session 2 Pre-Quiz

**1. Which file format is used to store the coordinates of the protein in GROMACS?**

**a) .itp**

**b) .top**

**c) .gro**

**d) .mdp**

**2. Which ensemble simulates a system with a constant number of particles, constant temperature, and constant pressure?**

**a) Microcanonical (NVE) ensemble**

**b) Canonical (NVT) ensemble**

**c) Isothermal-isobaric (NPT) ensemble**

**d) Grand Canonical (μVT) ensemble**

**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. In molecular dynamics, what does the term “force field” refer to?**

a) A region in space where forces are negligible

b) A mathematical model describing the forces between particles

c) An electromagnetic field surrounding a molecule

d) A graphical representation of molecular orbitals

**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 produce a plot of pressure evolution during the simulation?**

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