Session 2 Quiz

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

a) Increase the system’s temperature

b) Minimise the forces acting on each atom

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

This is hard. Can we do another ensemble question? See Q suggestions below. Also would be good to have a more theory one on what is MD/why MD.

**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) Evolution of the protein structure over simulation time

c) Solvent interactions with a folded protein

d) The electrical charge distribution within the protein

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

a) Energy minimization efficiency

b) Protein compactness and stability of its 3D-structure (felt folding state was a bit ambiguous – mb I m wrong)

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 group

**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

not too keen on this one – may be swap for one below?

**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

**Qs suggestions:**

**(could use for the pre-Q)**

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

1. .itp
2. .top
3. .gro
4. .mdp

**(very similar to the pre-Q)**

**Which ensemble is used to simulate a system with a constant number of particles, constant temperature, and constant volume?**

1. Microcanonical (NVE) ensemble
2. Canonical (NVT) ensemble
3. Isothermal-isobaric (NPT) ensemble
4. Grand Canonical (μVT) ensemble

**(or make one of the options of the NVT a bit madder:)**

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

1. Constant number of particles, volume and temperature
2. Normalized Velocity Trajectory
3. Number of molecules, Velocity, Temperature
4. Number, Volume, Trajectory

**(I think this one is a good general MD one and we should have one of these in each part of quiz )**

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

1. Density of molecular system under given conditions
2. Colour changes in chemical reactions
3. Electronic structure of a photochemically excited molecule
4. All of the above