Modeling questions (True/False)

1. In a molecular dynamic simulation:
   a) Temperature has no importance.
   b) The higher the temperature the more the system goes toward the local minima.
   c) Temperature is always fixed at 300K.
   d) The higher the temperature the more the system explores different conformations.

2. In a molecular dynamic simulation, interactions between atoms:
   a) Are computed on the basis of quantum mechanics and derive from first principles.
   b) Are computed through effective potentials that try to reproduce some molecular properties.
   c) Are established universally and they are the same for all systems.
   d) Include nuclear interaction.

3. In a molecular dynamic simulation, particles interactions:
   a) Are always repulsive.
   b) Are always attractive, but thanks to the temperature they can escape this attraction.
   c) Always include a repulsive component representing the effect of the volume occupied by the particle.
   d) Can change during the course of the simulation.

4. In a molecular dynamic simulation:
   a) Newton's second equation F=ma is used to compute particles trajectories due to interaction potentials.
   b) Particles velocities are proportional to the force acting on them.
   c) Positions and velocities are obtained from integration of acceleration.
   d) There is only one force acting on any given particle.

5. In a molecular dynamic simulation, bonded interactions represent:
   a) Electrostatic interactions between neighboring particles.
   b) Hydrogen bonds, setting an equilibrium distance and the bond geometry through angles and torsions.
   c) The interaction between atoms nuclei.
   d) Covalent bonds, setting an equilibrium distance and the bond geometry through angles and torsions.

Physics questions (True/False)

1. The interaction between two atoms depend only on their distance and it is described by a potential of the form:

$$U(d) = U_0 \left(\frac{a^3}{d^3} - \frac{a^2}{d^2} \right)$$

where d is the distance.
What is the equilibrium distance of the two atoms is U_0 = 1eV and a = 0.2nm?

2. An object is suspended by a spring in a gravitational field:
   a) The amplitude of the oscillations increases.
   b) The frequency of the oscillations increases.
   c) The equilibrium position shifts upward.
   d) The equilibrium position shifts downward.

3. Two particles are charged +2e and -e respectively:
   a) The two particles can be placed in an equilibrium position.
   b) The two particles can form an ionic bond.
   c) The two particles can form a hydrogen bond.
   d) The most important interaction is the dipole interaction.

4. If, at a given time t, the total force acting on every particle of the system is zero:
   a) The conformation adopted by the system will remain the same all following times.
   b) If the velocity of each particle is zero at time t, it will remain zero at all following times.
   c) The system is at equilibrium.
   d) The energy of the system is zero.

5. In a dissipative system:
   a) The total energy of the system and its environment is not conserved.
   b) The number of particles is not conserved.
   c) The system looses energy through heat.
   d) The system will end up in it global energy minimum.

6. Two molecules interact through a harmonic potential whose equilibrium distance is equal to a.
   a) If the temperature increases the frequency of oscillations around the equilibrium position increases as well.
   b) If temperature increases the amplitude of the oscillations around the equilibrium position increases as well.
   c) It is possible to break the interaction by raising the temperature.
   d) If the temperature decreases the molecules come into closer contact.

7. If a system of harmonic oscillators is at temperature T,
   a) The average kinetic energy and the potential energy are proportional to T.
   b) The average potential energy is equal to zero.
   c) If the energy is sufficiently high the particles become free.
   d) The average global energy of the system decreases with time.

8. The following diagram represents the potential energy U between two molecules as a function of their distance x.
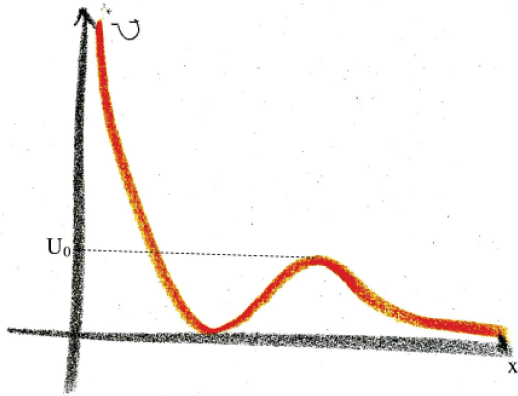

   a) The molecules can't be bound.
   b) The molecules can't be separated.
   c) The molecules are bound if their total energy is less than U_0.
   d) The molecules are not bound if their total energy is greater than U_0.

Chemistry questions (True/False)

1. The spatial arrangement of a biopolymer is a consequence of:
    a) the equilibrium between the local interactions of the backbone and the electrostatic interactions of the backbone.
    b) its secondary structures.
    c) the equilibrium between covalent interactions, electrostatic interactions and interactions with the solvent.
    d) the shape of the atomic orbitals of the atoms composing the molecule.

2. The shape of a small molecule is a consequence of:
    a) the shape of the most internal orbitals of the atoms composing the molecule.
    b) the shape of the valence orbitals of the atoms composing the molecule.
    c) the equilibrium between the repulsion of nuclei and the attraction of the electrons with the nuclei.
    d) the electronegativity of the atoms composing the molecule.

3. The interactions characteristic of biomolecules giving rise to secondary structures in proteins and nucleic acids are:
    a) Hydrophobic interactions.
    b) Van der Waals forces.
    c) Coulomb electrostatic interactions.
    d) Hydrogen bonds.

4. Because of the interactions with the solvent, a protein with many hydrophobic residues, in the water will have the tendency to:
    a) Fold in a globular shape.
    b) Remain unfolded.
    c) Form many hydrogen bonds.
    d) Adopt an elongated shape.

5. A single stranded RNA:
    a) Always folds in a double helix.
    b) Remains unfolded because it can't have perfectly complementary bases.
    c) Folds to form structures minimizing the interaction energies between its constituents.
    d) Can form complex structures that depend on the specific sequence and that can involve non-canonical pairings.

6. An RNA molecule is placed in a solution rich in positives ions.
    a) The strongest interactions (dominant) between portions of the molecule far way from each other are dipolar interactions.
    b) Molecules will be surrounded by an ionic cloud of positives ions to neutralize the negative charge of the phosphate groups.
    c) Coulomb's electrostatic interaction will be stronger at long distances because it will be amplified by the presence of the ions in solution.

d) The molecule will be surrounded by an ionic cloud of positives ions to neutralize the negative charge of the bases.

7. Looking at the chemical structure of the RNA bases, we can assert that:

Nitrogenous Bases of RNA
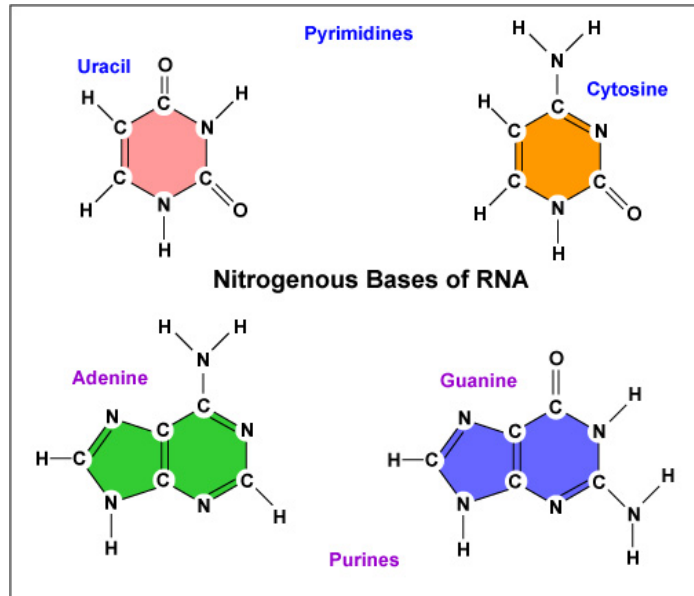
a) There is only one possibility for base pairing: G with C and A with U.
b) Bases can all pair with one another, two at the time.
c) Bases can all pair with one another with the possibility for a base to be paired with two others.
d) There are multiple base pairings possible, but they always involve a purine paired with a pyrimidine.

8. X-ray crystals of nucleic acids always reveal the presence of Mg++ ions near the molecule. This explains because:
   a) The ions form dipolar interactions with the molecule.
   b) The ions form hydrogen bonds with the molecule.
   c) The ions interact with the bases, which are negatively charged in solution.
   d) The ions interact with the oxygen atoms of the phosphate groups, which are negatively charged in solution.

9. If a DNA helix is placed in a heat bath, as we raise the temperature the following phenomena are observed.
   a) Base pairs break and the helix opens.
   b) Molecular vibrations intensify.
   c) The backbone of the molecule breaks.

What is the order in which these three phenomena occur as the temperature is raised?