Exercises – Lecture 10
BIO-212

Question 1

The two accessible conformations of a protein differ by 2 kJ/mol. What percentage of proteins will be in the higher energy state at 270 K?

Question 2

The Boltzmann distribution describes the most probable distribution of particles in different energy states for a given system. Thinking about each particle as being a protein and remembering that each different possible conformation of a protein has a different energy, use the Boltzmann distribution to explain why at extremely high temperatures proteins are unfolded.

Question 3

A protein can transition between two conformations which differ by 5 kJ/mol. Which of the following statements is false?

a. 15 % of the protein is in the higher energy state at 350 K
b. 10 % of the protein is in the higher energy state at 270 K
c. The protein can change conformation at room temperature
d. 90 % of the protein is in the lower energy state at 300 K

Question 4

A particular sidechain has a dihedral angle for which the energy is governed by the following equation:

$$U_{\mathrm{dihedral}} = 2 \times \cos(3 \times angle) \text{ kJ/mol}$$

A. What is the torsional energy of the sidechain when the angle is 60 °?

B. And when the angle is 120°?

C. What is the relative population of sidechains with an angle of 60 ° vs 120 ° at 300 K?

D. Would it be possible to visit a state with a dihedral angle of 180° at 300 K, given that the initial dihedral angle is 60°? Explain your answer considering possible energy barriers.

Question 5

The energy associated a specific torsional angle of a given molecule can be described by thefollowing potential: $U(\vartheta) = U_0\ (1 + \cos 4\ \vartheta)$ with $U_0 = 6$ kJ/mol. Which of the following statements is false?

a. The maximum energy value associated with the interaction is 12 kJ/mol
b. The torsional angle has 4 possible minima
c. At the minima the energy is zero
d. The minimal amount of energy required to jump between two minima is 6 kJ/mol

Question 6

A system at 275 K in state A has an enthalpy of –25 kJ and an entropy of 2 J•K^{-1}. In state B, it has an enthalpy of –20 kJ and an entropy of 10 J•K^{-1}. Will state A convert spontaneously to state B?

	State A	State B
H	–25 kJ	–20 kJ
S	2 J•K–1	10 J•K–1

Question 7

Assume that entropy and enthalpy changes are independent of temperature. A system in state A has an enthalpy of –22 kJ and an entropy of 7 J•K^{-1}. In state B, it has an enthalpy of –12 kJ and an entropy of 15 J•K^{-1}. At what temperatures will state B be favored?

	State A	State B
H	−22 kJ	−12 kJ
S	7 J•K−1	15 J•K−1

Question 8

The potential energy between two atoms is described by a **Lennard-Jones potential**:

$$U_{VdW} = \sum_{i>j}^{N} \epsilon \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - 2 \left(\frac{r_0}{r_{ij}} \right)^{6} \right]$$

Given:

- ϵ=2 kJ/mol,
- r_0=0.4 nm

a) Calculate the potential energy U(r) at r=0.45 nm.

b) At what distance r is the potential energy at its minimum?

c) Choose the correct interpretation of the potential:

- The term $(\frac{r_0}{r})^{12}$ describes the attractive force.
- The term $(\frac{r_0}{r})^{6}$ describes the repulsive force.
- The potential U(r) accounts for both attractive and repulsive interactions.
- The distance r = r_0 corresponds to the strongest attractive force.

Question 9

During cellular respiration, a glucose molecule is gradually broken down into carbon dioxide and water. Below you have a reaction:

$$C_6H_{12}O_6(\text{glucose}) + 6\,O_2(\text{gas}) \rightarrow 6\,CO_2(\text{gas}) + 6\,H_2O(\text{liquid})$$

Using a table from the lecture:

Compound	$\Delta G^{\circ\prime}$ (kJ•mol^{-1})
acetate$^-$	−369.2
CO_2 (gas)	−394.4
CO_2 (aqueous solution)	−386.2
carbonate ion	−587.1
ethanol	−181.5
fructose	−915.4
fructose-6-phosphate^{2-}	−1758.3
α-D-glucose	−917.2
glucose-6-phosphate^{2-}	−1760.2
H^+ (aqueous solution)	0.0
H_2 (gas)	0.0
H_2O (liquid)	−237.2
isocitrate^{3-}	−1160.0
lactate$^-$	−516.6
OH^-	−157.3
pyruvate$^-$	−474.5
succinate^{2-}	−690.2

a) Calculate the standard Gibbs free energy change (ΔG) for the reaction

b) Interpret the result: Is the reaction thermodynamically favorable under standard conditions?

<u>Question 10:</u>

In the lecture you had 2 pathways (1) ans (2) on the picture below.
Check what would be the Gibbs energy for both. Use the table from question 10. What you can say?