

CHEM-E3150 Biophysical chemistry. Exam 20.02.2020.

Please answer all 5 questions (including possible a, b, and c-parts). Calculators are allowed. No other materials allowed. On page 2 there is a list of possibly useful equations and relations. Show clearly how you came to your conclusions.

1. The free concentration of a ligand was kept constant at $1 \cdot 10^{-7}$ M. It is bound to a receptor A with a K_D of 1 nM, and to another receptor B with a K_D of 1 μ M.

- What is the ratio of the fractional occupancies of the receptors?
- Draw a graph of the fractional occupancies that illustrates the situation.
- What happens if we increase the concentration of receptor A to the double?

2. A system with 100 000 molecules has two energy levels (A and B). At first, the two energy levels are populated equally. After a reversible process, energy level A is populated by 65% of the molecules and the system is at 293 K.

- What is the change in entropy?
- How much heat was added or removed from the system?

3. 1000 water molecules surround a hydrophobic particle. They are restricted in movement so that they can take only one of two available positions A or B. The probability of positions A and B are equal.

- What is the most likely distribution between the two positions?
- What is the multiplicity of this distribution? Solve using Stirling's approximation and express the result as a power of 10.
- What is the multiplicity of a case in which the 1000 water molecules could take any of five equally likely positions?

4. The unfolding of a protein was studied by differential scanning calorimetry (DSC). The melting temperature of the protein was 110 °C. The measured difference in heat capacity (at constant pressure) between the unfolded and folded protein ΔC_p was 3,21 kJK⁻¹mol⁻¹. The integrated peak area of denaturation in the melting curve, i.e. the heat of unfolding was 333,22 kJmol⁻¹.

- Draw as clearly as possible with the available data, a curve for the temperature dependence of the heat capacity.
- What would the entropy of unfolding be at 25 °C?
- How do the enthalpy and entropy components of the free energy of unfolding change with temperature for the protein?

5. Imagine proteins diffusing away from an initial sharp point.

- Draw a picture using the concept of a root-mean-square distance (RMSD) value to explain how the diffusion progresses over time. What determines the value of RMSD?
- At a distance of 30 μ m, how long time will it take until the probability of finding a protein is 50 % of what it is at the initial point? The diffusion coefficient is $1,11 \cdot 10^{-6}$ cm²s⁻¹ at 25 °C.

Some equations and relations that might be useful:

$$D = \frac{k_B T}{6\pi\eta r}$$

$$D = k_B T / f$$

$$\text{r.m.s. distance} = \sqrt{6Dt}$$

$$S = -Nk_B \sum_i p_i \ln(p_i)$$

$$[LR] = \frac{B_{max} * [L]}{K_D + [L]}$$

$$R = 8.314 \text{ JK}^{-1}\text{mol}^{-1}$$

$$k_B = 1.38 \times 10^{-23} \text{ JK}^{-1}$$

$$0 \text{ }^\circ\text{C} = 273 \text{ K}$$

$$p(x) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma} e^{-\frac{(x_{1/2} - \mu)^2}{2\sigma^2}}$$

$$\Delta G = \Delta H - T\Delta S$$

$$\Delta G^\circ = RT \ln K_D$$

$$\Delta S = q_{rev}/T$$

$$dH = C_p dT$$

$$F = fv$$

$$\mu = \mu^\circ + RT \ln C$$

$$S = k_B \ln W$$

$$W = M! / (N!(M-N)!)$$

$$n! = (n/e)^n$$

$$S_v = m_{eff}/f$$