BB 101: Physical Biology

TUTORIAL 4: Solutions

1. A freely-jointed chain tends to coil itself because it is trying to maximize entropy. The entropy of a macromolecular chain is dependent upon the number of different conformations that the chain can have in space (configurational entropy: S(r)=kB*ln(Ω). If the chain were totally stretched out, it would only have one possible conformation. By coiling itself, it increases the number of conformations it can have, and therefore, its entropy.

2. The expected RMS end-to-end distance for an ideal freely jointed chain of this length is b√N =30 Å. The "real" RMS (=100 Å) of this chain is greater than this number, Therefore, it does not behave as an ideal chain.

3. Bending stiffness k_b $= N\xi_p k_B T = \xi_p RT =$ 300 Å kcal mol^{-1}

4. Given

$$G = \langle U \rangle - TS$$

$$= \sum_i u_i p_i + k_B T \sum_i p_i ln p_i$$

$$= \sum_i p_i \{u_i + k_B T ln p_i\}$$

Now, use expression for p_i

$$= \sum_i \frac{1}{Z} e^{-\beta u_i} \left\{ u_i + k_B T ln \left(\frac{1}{Z} e^{-\beta u_i} \right) \right\}$$

$$= \frac{1}{Z} \sum_i e^{-\beta u_i} \{u_i - k_B T ln\, Z - u_i\}$$

$$= \frac{1}{Z} \sum_i e^{-\beta u_i} \{-k_B T ln\, Z\}$$

$$= \frac{Z}{Z} \{-k_B T ln\, Z\}$$

Therefore, $G = -k_B T ln\, Z$

5. Given

$$U_i = \sum_{l=1}^{2} \sum_{m=l+1}^{3} \frac{A}{r_{lm}}$$

$$= \sum_{2}^{3} \frac{A}{r_{1m}} + \sum_{3}^{3} \frac{A}{r_{2m}}$$

$$= \frac{A}{r_{12}} + \frac{A}{r_{13}} + \frac{A}{r_{23}}$$

(a) Energy of any straight conformation/microstate

$$U_s = \frac{A}{r_{12}} + \frac{A}{r_{13}} + \frac{A}{r_{23}}$$

$$= \frac{1\ k_B T\ nm}{1\ nm} + \frac{1\ k_B T\ nm}{2nm} + \frac{1\ k_B T\ nm}{1nm}$$

$$= 2.500\ k_B T$$

(b) Energy of any bent conformation/microstate

$$U_b = \frac{A}{r_{12}} + \frac{A}{r_{13}} + \frac{A}{r_{23}}$$

$$= \frac{1\ k_B T\ nm}{1\ nm} + \frac{1\ k_B T\ nm}{\sqrt{2}\ nm} + \frac{1\ k_B T\ nm}{1nm}$$

$$= 2.707\ k_B T$$

(c) There are total 6 straight conformations/microstates possible i.e. $W_s = 6$

(d) There are total 16 bent conformations/microstates i.e. $W_b = 16$

The probability P_s that you will find the protein in a straight structural state or straight macrostate is given by

$$P_s = \frac{e^{-\frac{G_s}{k_B T}}}{Z}$$

Where $G_s = \langle U_s \rangle - TS = \langle U_s \rangle - T k_B\ lnW_s$

And, $\langle U_s \rangle$ is average energy of straight microstates is, W_s is the number of straight microstates and Z is the partition function

Similarly, probability P_b that you will find the protein in a bent structural state or bent macrostate is given by

$$P_b = \frac{e^{-\frac{G_b}{k_B T}}}{Z}$$

$$G_b = \langle U_b \rangle - TS = \langle U_b \rangle - T k_B \; lnW_b$$

Where $\langle U_b \rangle$ is average energy of bent microstates

$$Z = e^{-\frac{G_S}{k_B T}} + e^{-\frac{G_b}{k_B T}}$$

Now, $\quad G_s = 2.500\, k_B T - k_B\, T\, ln6 = 2.500\, k_B T - 1.792\, k_B\, T \quad = \quad 0.708\, k_B T$

And, $\quad G_b = 2.707\, k_B T - k_B\, T\, ln16 = 2.707\, k_B T - 2.773\, k_B\, T = -0.066\, k_B T$

(e) The probability that you will find the protein in a straight structural state or straight macrostate is given by

$$P_s = \frac{e^{-0.708}}{e^{-0.708} + e^{0.066}} = \frac{e^{-0.708}}{e^{-0.708} + e^{0.066}}$$

≈0.316

(f) The probability that you will find the protein in a bent structural state or bent macrostate is given by

$$P_b = \frac{e^{0.066}}{e^{-0.708} + e^{0.066}} = \frac{e^{0.066}}{e^{-0.708} + e^{0.066}}$$

≈0.684

6. (a) Let's calculate entropy/disorder S_1 for first column

For this column M=1, Since nothing is changing in first column

Here p_1 is the probability of finding letter A

$$p_1 = 1$$

Therefore, $S_1 = -k_B p_1 \ln p_1 = -k_B \ln 1 = 0$

Now, let's calculate entropy S_2 for second column

For this column M=4, since there are four different letters in this position.

Let p_1,p_2, p_3 and p_4 denote the probabilities of finding letters A, T, C and G respectively

$$p_1 = \frac{2}{10} = 0.2$$

$$p_2 = \frac{3}{10} = 0.3$$

$$p_3 = \frac{2}{10} = 0.2$$

$$p_4 = \frac{3}{10} = 0.3$$

Therefore, $$S_2 = -k_B(p_1 \ln p_1 + p_2 \ln p_2 + p_3 \ln p_3 + p_4 \ln p_4)$$

$$S_2 = -k_B(-1.366)$$

Or, $$S_2 = 1.366k_B$$

Now, Let's calculate entropy $S_3$for third column

For this column M=4, Since there are four different letters in this position

Letp_1,p_2, p_3 and p_4 denote the probabilities of finding letters A, T, C and G respectively

$$p_1 = \frac{1}{10} = 0.1$$

$$p_2 = \frac{7}{10} = 0.7$$

$$p_3 = \frac{1}{10} = 0.1$$

$$p_4 = \frac{1}{10} = 0.1$$

Therefore, $$S_3 = -k_B(p_1 \ln p_1 + p_2 \ln p_2 + p_3 \ln p_3 + p_4 \ln p_4)$$

$$S_3 = -k_B(-0.94)$$

Or, $$S_3 = 0.94\ k_B$$

(b) Since Values of entropy is minimum for first column and hence first position is most conserved. Second position is least conserved as entropy is maximum for this position.