BB 101: Physical Biology

TUTORIAL 3: Solutions

1. (i) Partition function

$$Z = e^{-\frac{\epsilon_1}{k_B T}} + e^{-\frac{\epsilon_2}{k_B T}} + e^{-\frac{\epsilon_3}{k_B T}}$$

$$= e^{-\frac{0}{4.14}} + e^{-\frac{4.14}{4.14}} + e^{-\frac{8.28}{4.14}}$$

$$= e^{-0} + e^{-1} + e^{-2}$$

$$= 1 + 0.368 + 0.135$$

$$= 1.503$$

(ii) Average separation $\langle l \rangle$ is given by

$$\langle l \rangle = \sum_{i=1}^{i=3} p_i l_i$$

Now,

$$p_1 = \frac{e^{-\frac{\epsilon_1}{k_B T}}}{Z} = \frac{e^{-0}}{Z} = \frac{1}{1.503} = 0.665$$

$$p_2 = \frac{e^{-\frac{\epsilon_2}{k_B T}}}{Z} = \frac{e^{-1}}{Z} = \frac{0.368}{1.503} = 0.249$$

$$p_3 = \frac{e^{-\frac{\epsilon_3}{k_B T}}}{Z} = \frac{e^{-2}}{Z} = \frac{0.135}{1.503} = 0.090$$

Therefore,

$$\langle l \rangle = 0.665 \times 1 + 0.249 \times 1.5 + 0.090 \times 2.0$$

$$= 0.665 + 0.374 + 0.180$$

$$= 1.219 \text{ Å}$$

(iii) Average energy of the loop $\langle \epsilon \rangle$ is given by

$$\langle \epsilon \rangle = \sum_{i=1}^{i=3} p_i \epsilon_i$$

,

$$= 0.665 \times 0 + 0.249 \times 4.14 + 0.090 \times 8.28$$

$$= 0 + 1.031 + 0.745$$

$$= 1.776\ pN\ nm$$

2. 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 $G_s = \langle U_s \rangle - TS = \langle U_s \rangle - T k_B\ ln W_s$

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

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

$$G_b = \langle U_b \rangle - TS = \langle U_b \rangle - Tk_B\ lnW_b$$

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

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

(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

3. $S = -k \sum_i p_i\ lnp_i$

For a single macrostate when energies of all micro-states are identical then

$$p_i = \frac{1}{w}$$

Therefore,

$$S = -k \sum_i \frac{1}{w} ln \frac{1}{w}$$

Or, $$S = -k\frac{1}{w}\sum_i ln\frac{1}{w}$$

$$= -k\frac{1}{w}\sum_i \ln[w]^{-1}$$

$$= k\frac{1}{w}\sum_i \ln\mathrm{w}$$

$$= k\frac{w}{w}\ln\mathrm{w}$$

$$= k\ln\mathrm{w}$$

4. (i) 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, $$S_3 = 0.94\ k_B$$

(ii) 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.