BB 101: Module II

TUTORIAL 4: Solutions

1. 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. $W_b = 6$

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

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

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

≈0.684

2. (a) In this case $\frac{\partial \rho}{\partial t}$ will be proportional to the fraction of empty sites

Therefore, $\frac{\partial \rho}{\partial t} \propto (1 - \rho)$

Or, $\frac{\partial \rho}{\partial t} = k^+ \,(1 - \rho)$

Integrate above equation to obtain how mean density ρ changes with time with initial condition that $\rho = 0$ at $t = 0$

Therefore, $\int_0^{\rho} \frac{d\rho}{(1-\rho)} = k^+ \int_0^{t} \mathrm{dt}$

Or, $[-ln(1-\rho)]_0^{\rho} = k^+[t]_0^t$

Or, $[ln(1-\rho)]_0^{\rho} = -k^+[t]_0^t$

Or, $ln(1-\rho) - \ln 1 = -\, k^+t$

Or, $ln(1-\rho) = -k^+t$

Or, $(1-\rho) = e^{-k^+t}$

Or, $\rho = 1 - e^{-k^+t}$

(b) In this case $\frac{\partial \rho}{\partial t}$ will be proportional to the fraction of occupied sites

Therefore, $\frac{\partial \rho}{\partial t} \propto \rho$

Or, $\frac{\partial \rho}{\partial t} = -k^- \,\rho$

Integrate above equation to obtain how mean density ρ changes with time with initial condition that $\rho = 1$ at $t = 0$

Therefore, $\int_1^{\rho} \frac{d\rho}{\rho} = -k^- \int_0^{t} \mathrm{dt}$

Or, $[ln\rho]_1^{\rho} = -k^-[t]_0^t$

Or, $ln\rho - \ln 1 = -\, k^-t$

Or, $ln\rho = -k^-t$

Or, $\rho = e^{-k^-t}$

(c) In this case $\frac{\partial\rho}{\partial t} = k^+\,(1-\rho) - k^-\,\rho$

(d) In steady state $\frac{\partial\rho}{\partial t} = 0$

Therefore, $k^+\,(1-\rho) - k^-\,\rho = 0$

This implies that

$$\rho = \frac{k^+}{k^+ + k^-}$$

(e) (i) $k^+ = k^- \Rightarrow \qquad \rho = \frac{k^+}{k^+ + k^+} = \frac{1}{2}$

(ii) $k^+ = 2k^- \Rightarrow \qquad \rho = \frac{2k^-}{2k^- + k^+} = \frac{2}{3}$

(iii) $k^- = 2k^+ \Rightarrow \qquad \rho = \frac{k^+}{k^+ + 2k^+} = \frac{1}{3}$

(iv) $k^+ = 0 \Rightarrow \qquad \rho = \frac{0}{0 + k^-} = 0$

(v) $k^- = 0 \Rightarrow \qquad \rho = \frac{k^+}{k^+ + 0} = 1$

3. Given $\qquad S = -K \sum_i \; p_i \ln p_i$

$$\Rightarrow \qquad S = -k_B \sum_i \; p_i \ln p_i$$

Or, $S = -k_B \sum_i \; p_i \ln p_i$

Given $p_i = \frac{1}{Z} e^{-\frac{U_i}{k_B T}} = \frac{1}{Z} e^{-\beta U_i}$ $\qquad$ where $\beta = \frac{1}{k_B T}$

Therefore, $\qquad S = -k_B \sum_i \; \{\frac{1}{Z} e^{-\beta U_i}\} \ln\{\frac{1}{Z} e^{-\beta U_i}\}$

Or, $$S = -k_B \sum_i \left\{\frac{1}{Z} e^{-\beta U_i}\right\}\{-\beta U_i - \ln Z\}$$

Or, $$S = k_B \beta \sum_i \left\{\frac{1}{Z} e^{-\beta U_i}. U_i\right\} + k_B \sum_i \{\frac{1}{Z} e^{-\beta U_i} \ln Z\}$$

Or, $$S = \frac{k_B}{k_B T} \sum_i \left\{\frac{1}{Z} e^{-\beta U_i}. U_i\right\} + k_B \sum_i \{\frac{1}{Z} e^{-\beta U_i} \ln Z\}$$

Or, $$S = \frac{1}{T} \sum_i \{p_i. U_i\} + k_B \frac{\ln Z}{Z} \sum_i \{e^{-\beta U_i}\}$$

Or, $$S = \frac{\langle U \rangle}{T} + k_B \frac{\ln Z}{Z} \mathrm{Z}$$

$$S = \frac{\langle U \rangle}{T} + k_B \ln Z$$

Now use $-k_B T \ln Z = G$

$$S = \frac{\langle U \rangle}{T} - \frac{G}{T}$$

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

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

4. (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_2, 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

Let p_2, 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 at entropy is maximum for this position.