

Physis 187

①

Homework #4 Solutions

1. Jackson 5.1

Derive: $K_T Y_1 = K_R Y_0$

Using $K_T = \frac{[T_1]}{[T_0][L]}$, $K_R = \frac{[R_1]}{[R_0][L]}$, $Y_0 = \frac{[R_0]}{[T_0]}$

$$Y_1 = \frac{[R_1]}{[T_1]}$$

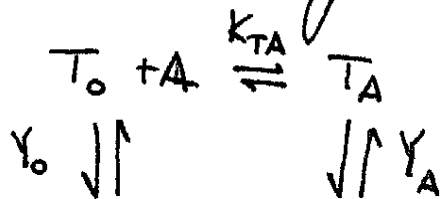
From here $K_T Y_1 = \frac{[T_1]}{[T_0][L]} \cdot \frac{[R_1]}{[T_1]} = \frac{[R_1]}{[T_0][L]}$

$$K_R Y_0 = \frac{[R_1]}{[R_0][L]} \cdot \frac{[R_0]}{[T_0]} = \frac{[R_1]}{[T_0][L]}$$

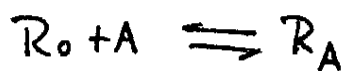
So $K_T Y_1 = K_R Y_0$.

3. Use energy balance to express Y_0 or Y_{AB} in terms of the binding constants

A B binding scheme

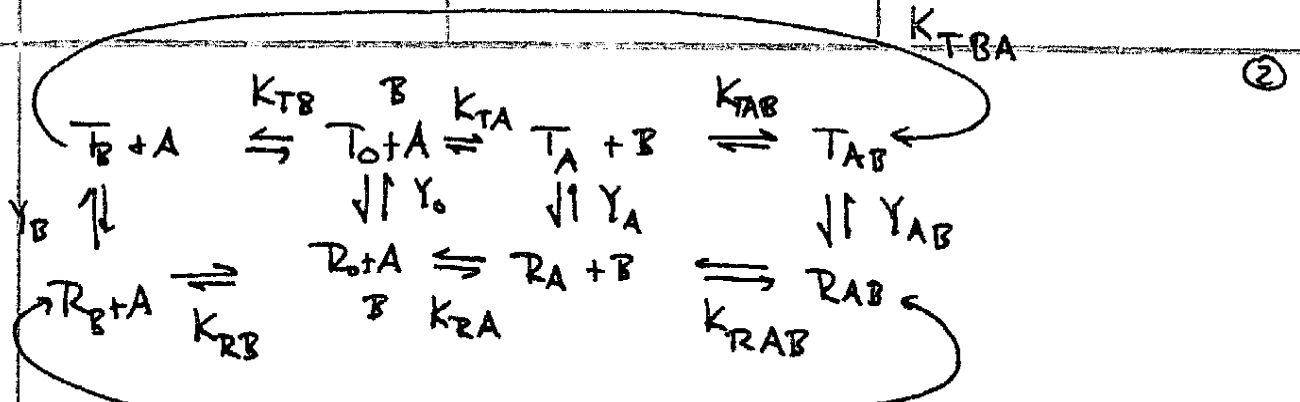


and the same for B.



To put these together we need a

new picture.



Anyway, for our calculation we need to consider two paths

$$\begin{aligned}
 & RT \log Y_0 + RT \log K_{RA} + RT \log K_{RAB} \\
 &= RT \log K_{TA} + RT \log K_{TAB} + RT \log Y_{AB}
 \end{aligned}$$

$$\Rightarrow Y_0 K_{RA} K_{RAB} = Y_{AB} K_{TA} K_{TAB}$$

$$\boxed{\frac{Y_0}{Y_{AB}} = \frac{K_{TA} K_{TAB}}{K_{RA} K_{RAB}}}$$

4. In the MWC model find the fraction of R-state protein as a function of $[L]$.

$$A = \frac{\sum_{i=0}^n [R_i]}{\sum_{i=0}^n ([R_i] + [T_i])}$$

we already derived (see class notes)

$$\sum_{i=0}^n [R_i] = [R_0] [1 + K_R [L]]^n$$

$$\sum_{i=0}^n [T_i] = [T_0] [1 + K_T [L]]^n$$

$$A = \frac{[P_0] (1 + K_R [L])^n}{[P_0] (1 + K_R [L])^n + [T_0] (1 + K_T [L])^n}$$

or

$$A = \frac{Y_0 (1 + K_R [L])^n}{Y_0 [1 + (K_R [L])^n] + (1 + K_T [L])^n}$$

5. Show that the above result goes to Eq. 5.4 when $n=1$


$$A_{n=1} = \frac{1 + K_R [L]}{1 + K_R [L] + \frac{1}{Y_0} (1 + K_T [L])}$$

But $K_T Y_1 = K_R Y_0$

$$A_{n=1} = \frac{1 + K_R [L]}{1 + K_R [L] + \frac{1}{Y_0} (1 + \frac{K_R Y_0 [L]}{Y_1})}$$

$$= \frac{1 + K_R [L]}{(1 + Y_0^{-1}) + [L] K_R (1 + Y_1^{-1})} \leftarrow \text{Eq. 5.4 checks}$$

9. Derive the KNF binding curve for a dimer.

We have  Following the class notes p. 59

$$\frac{[P_1]}{[P_0][L]} = e^{-\Delta G/RT} = 2 K_S \sigma$$

↑
two half-filled states.

$$\frac{[P_2]}{[P_1][L]} = \frac{1}{\sigma} K_S \frac{1}{2} \leftarrow \text{lose entropy}$$

↑
remove domain wall

$$[P_1] = [P_0][L] 2k_s \sigma$$

$$[P_2] = \frac{1}{2\sigma} k_s [P_1][L] = [P_0][L]^2 k_s^2$$

Binding curve \Rightarrow

$$B = \frac{[P_1] + 2[P_2]}{2\{[P_0] + [P_1] + [P_2]\}}$$

$$B = \frac{[P_0][L] 2k_s \sigma + 2[P_0][L]^2 k_s^2}{2\{[P_0] + [P_0][L] 2k_s \sigma + [P_0][L]^2 k_s^2\}}$$

$$B = \frac{k_s \sigma [L] + [L]^2 k_s^2}{1 + 2k_s \sigma [L] + [L]^2 k_s^2}$$

for large σ : $B \cong \frac{k_s \sigma [L]}{2k_s \sigma [L] + [L]^2 k_s^2}$

$$\Rightarrow B \cong \frac{1}{2} \frac{1}{1 + [L](k_s/2\sigma)}$$

\nwarrow effective binding constant for the second ligand.

for σ large and $[L]$ small.

$$k_s \sigma [L] \ll 1$$

$$B \cong \frac{k_s \sigma [L]}{1 + 2k_s \sigma [L]} \checkmark$$

5.  Remember periodic bc.

How many states are there?

P_0	— — — —	1 way	Domain walls 0
P_1	— — — X	4 ways	1
P_2	— X — X	2 ways	2
P_2'	— — X X	4 ways	1
P_3	X X X —	4 ways	1
P_4	X X X X	1 way	0

Total of $2^4 = 16$ states.

$$\frac{[P_1]}{[L][P_0]} = \frac{4 K_s \sigma}{1} \quad \frac{[P_2]}{[L][P_1]} = \frac{2 K_s^2 \sigma^2}{4}$$

and $\frac{[P_2']}{[L][P_1]} = \frac{4 K_s^2}{4} \quad \frac{[P_3]}{[L][P_2]} = \frac{4 K_s^2}{2 \sigma}$

$$\frac{[P_4]}{[L][P_3]} = \frac{1}{4 \sigma} K_s$$

Solve for all concentrations:

$$[P_1] = 4 K_s \sigma [L][P_0]$$

$$[P_2] = \frac{1}{2} K_s \sigma [L]^2 4 K_s \sigma [P_0] = 2 K_s^2 \sigma^2 [L]^2 [P_0]$$

$$[P_2'] = K_s [L][P_1] = 4 K_s^2 \sigma [L]^2 [P_0]$$

$$[P_2] = \frac{2}{\sigma} K_s [L] [P_2] = \frac{2}{\sigma} K_s [L]^2 (2 K_s^2 \sigma^2 [P_0]) [L]^2$$

$$[P_3] = 4 K_s^3 \sigma^2 [P_0] [L]^3$$

$$[P_4] = \frac{1}{4\sigma} K_s 4 K_s^3 \sigma [P_0] [L]^3 [L] = K_s^4 [L]^4 [P_0]$$

Bridij ana:

$$B = \frac{[P_1] + 2([P_2] + [P_2']) + 3[P_3] + 4[P_4]}{4\{[P_0] + [P_1] + [P_2] + [P_2'] + [P_3] + [P_4]\}}$$

$$B = \frac{4K_s^4 + 4K_s \sigma L P_0 + 4K_s^2 \sigma^2 L^2 P_0 + 8K_s^2 \sigma L^2 P_0 + 12K_s^3 \sigma P_0 L^3}{4\{ \quad \quad \quad \}}$$

$$B = \frac{K_s \sigma [L] + K_s^2 (\sigma^2 + 2\sigma) [L]^2 + 3 K_s^3 \sigma [L]^3 + K_s^4 [L]^4}{1 + 4 K_s \sigma [L] + 2 K_s^2 (\sigma^2 + 2\sigma) [L]^2 + 4 K_s^3 \sigma [L]^3 + K_s^4 [L]^4}$$