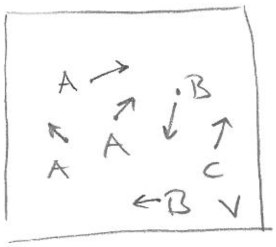
10/1/2010

1. MASS ACTION KINETICS

From the quiz:

$A + B \xrightarrow{k} C$



N_A: # A

N_B: # B

$c\,dt$: Prob. for reaction of one specific ~~molecule~~ pair in dt

$$dN_A = dN_B = -N_A \cdot N_B \cdot c\,dt$$

concentration of A: $[A] = N_A / V$

Unit: Mole/l (1 Mole $= 6.02 \cdot 10^{23}$ molecules)

$$\frac{dN_A}{V} = \frac{dN_B}{V} = -\frac{N_A \cdot N_B}{V^2}(cV\,dt) \; ; \; k = cV$$

$$\frac{d[A]}{dt} = \frac{d[B]}{dt} = -k[A][B] = -\frac{d[C]}{dt}$$

EXAMPLES:

(i) $A \xrightarrow{k} B$ $\quad d[A]/dt = -d[B]/dt = -k[A]$ (unimolecular)

(ii) $A + B \xrightarrow{k} C + D$ $\quad d[A]/dt = -k[A][B]$ (bimolecular)

(iii) $A + B \xrightarrow{k} A + C$ $\quad d[A]/dt = 0$ (catalytic)

$$d[B]/dt = -d[C]/dt = -k[A][B]$$

(iv) $A + B \xrightarrow{k} 2A$ (autocatalytic)

(v) $A \underset{k_-}{\overset{k_+}{\rightleftharpoons}} B$ (reversible)

Examples of chemical reaction equations

(i) DNA hybridization:

S: 5'-ACGTTCGA-3' : single-stranded DNA

$\bar{S}$: 5'-TCGAACGT-5' : complementary single strand

Watson-Crick base pairs: A=T, G≡T

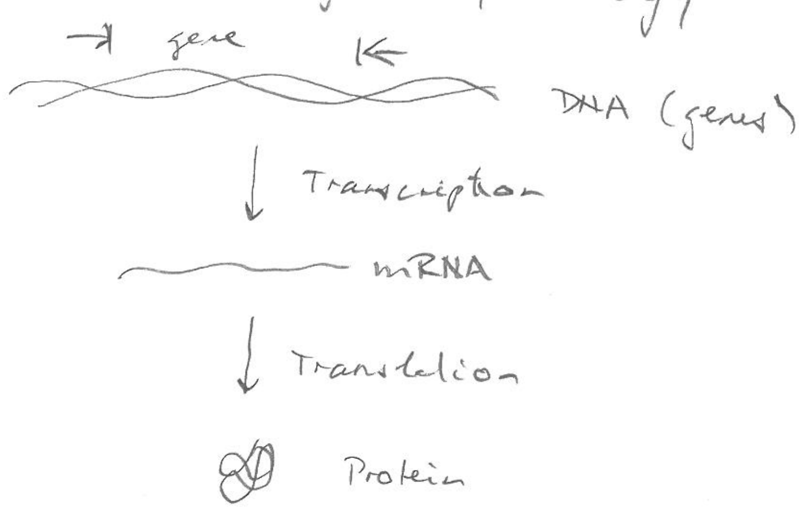
Hybridization: mix $S, \bar{S}$

5'-ACGTTCGA-3'
3'-TGCAAGCT-5' , $S\bar{S}$: double-stranded DNA (double helix)

What model would you use?

$$S + \bar{S} \xrightarrow{k} S\bar{S} \qquad \frac{d[S]}{dt} = -k[S][\bar{S}]$$

(ii) The central dogma of biology



$$D \xrightarrow{\alpha_m} D + m \quad \text{(transcription)}$$

$$m \xrightarrow{\alpha_P} m + P \quad \text{(translation)}$$

$$m \xrightarrow{\gamma_m} \emptyset$$

$$P \xrightarrow{\gamma_P} \emptyset$$

$$\frac{d[m]}{dt} = \alpha_m [D]^{\overset{1}{n}} - \gamma_m [m]$$

$$\frac{d[P]}{dt} = \alpha_p [m] - \gamma_p [P]$$

(iii) Bacterial growth

$$B \xrightarrow{k} 2B$$

$$B + F \xrightarrow{k} 2B \quad \text{(w/ resource constraints)}$$

(iv) Virus infection

$$B \xrightarrow{k_1} 2B$$

$$V + B \xrightarrow{k_2} 2V$$

$$V \rightarrow \emptyset$$

The language of chemical reactions can be used to model a large set of behaviors