Secret Code 20

8.2A) $\langle f_b \rangle = \frac{[MA]}{[M]+[MA]} = \frac{1}{\frac{[M]}{[MA]}+1} = \frac{1}{\frac{1}{[A]K_A}+1} = \boxed{\frac{[A]K_A}{1+[A]K_A}}$

$K_A = \frac{[MA]}{[M][A]} \quad [A]K_A = \frac{[MA]}{[M]} \quad \frac{1}{[A]K_A} = \frac{[M]}{[MA]}$

8.2B) $P = 1 + K_A[A] \qquad S = 1 \qquad \frac{\partial P}{\partial [A]} = K_A$

$\langle f_b \rangle = \frac{[A]}{SP}\frac{\partial P}{\partial [A]} = \frac{[A]}{S(1+K_A[A])} \cdot K_A = \boxed{\frac{K_A[A]}{1+K_A[A]}}$

8.2C) Python.

8.2D)

$$\begin{array}{ccc} M_0 & \overset{K_A}{\rightleftharpoons} & MA_1 \\ {\scriptstyle K_A}\downarrow\uparrow & & \downarrow\uparrow{\scriptstyle K_B} \\ MB_1 & \underset{K_A}{\rightleftharpoons} & MA_1B_1 \end{array} \Rightarrow P(A,B) = \frac{[M_0]}{[M_0]} + \frac{[MA_1]}{[M_0]} + \frac{[MB_1]}{[M_0]} + \frac{[MA_1B_1]}{[M_0]} = 1 + \left(\frac{[MA_1]}{[M_0]}\right) + \left(\frac{[MB_1]}{[M_0]}\right) + \left(\frac{[MA_1B_1]}{[M_0]}\right)$$

$$= 1 + [A]K_A + [B]K_B + [A][B]K_AK_B$$

$$\langle f_A \rangle = \frac{[A]}{SP}\left(\frac{\partial P(A,B)}{\partial [A]}\right)_B = \frac{[A]}{S \cdot P(A,B)} \cdot \left(K_A + [B]K_AK_B\right)$$

$S = 1$

$$= \boxed{\frac{[A]K_A + [A][B]K_AK_B}{1+[A]K_A+[B]K_B+[A][B]K_AK_B}}$$

$$\begin{array}{lll} M_0 + A \rightleftharpoons MA & \beta_{1,0} = K_A & K_A = \frac{[MA]}{[M_0][A]} \\ M_0 + B \rightleftharpoons MB & \beta_{0,1} = K_B & K_B = \frac{[MB]}{[M_0][A]} \end{array} \qquad K_{AB} = K_AK_B = \frac{[MAB]}{[M_0][A][B]}$$

$$M_0 + A \underset{}{\overset{K_A}{\rightleftharpoons}} MA_1 + B \overset{K_B}{\rightleftharpoons} MAB \qquad (K_AK_B)$$

8.2E) Python

8.2F)

$$\begin{array}{ccc} M_0 & \overset{K_A}{\rightleftharpoons} & MA \\ {\scriptstyle K_B}\downarrow\uparrow & & \\ MB & & \end{array}$$

$S = U = 1$

$$P(A,B) = \frac{[M_0]}{[M_0]} + \frac{[MA]}{[M_0]} + \frac{[MB]}{[M_0]} = 1 + K_A[A] + K_B[B]$$

$$\frac{\partial P(A,B)}{\partial [A]} = 0 + K_A + 0 = K_A$$

$M + A \rightleftharpoons MA : K_A = \frac{[MA]}{[M_0][A]}$

$M + B \rightleftharpoons MB \quad K_B = \frac{[MB]}{[M_0][B]}$

$$\langle f_A \rangle = \frac{[A]}{SP}\frac{\partial P(A,B)}{\partial [A]} = \frac{[A]}{1(1+[A]K_A+[B]K_B)} \cdot K_A = \boxed{\frac{K_A[A]}{1+[A]K_A+[B]K_B}}$$

8.3A) $\beta_i = \prod_{j=1}^{i} K_j$

$$\boxed{\begin{array}{ll} \beta_1 = K_1 = 10^2\ M^{-1} & \beta_3 = K_1K_2K_3 = 10^6\ M^{-3} \\ \beta_2 = K_1K_2 = 10^4\ M^{-2} & \beta_4 = K_1K_2K_3K_4 = 10^8\ M^{-4} \end{array}}$$

8.3B)

$$\left.\begin{array}{l} \beta_1 = K_1 = 10^4\ M^{-1} \\ \beta_2 = \beta_1K_2 = 10^6\ M^{-2} \\ \beta_3 = \beta_2K_3 = 10^7\ M^{-3} \end{array}\right\} \boxed{\begin{array}{l} K_1 = 10^4\ M^{-1} \\ K_2 = \frac{\beta_2}{\beta_1} = 10^2\ M^{-1} \\ K_3 = \frac{\beta_3}{\beta_2} = 10\ M^{-1} \end{array}}$$

8.3C) The system in part A has <u>no cooperativity</u>. The second binding step does not have a significantly larger stepwise constant than the first step

The system in part B has <u>negative cooperativity</u> because second binding step is 100 fold less favorable than the first.