Handout 8

Course equations

Interactions

$$u(r) = 4\epsilon\left[\left(\frac{r}{\sigma}\right)^{-12} - \left(\frac{r}{\sigma}\right)^{-6}\right]$$

Lennard-Jones

$$u(r) = \frac{q_1 q_2}{4\pi\epsilon_0 r}$$

Coulomb's law

Thermodynamics

$$S = k_B \ln \Omega \qquad \Delta S = \int \frac{\delta Q_{rev}}{T}$$

$$G \equiv U - TS + PV \qquad H \equiv U + PV \qquad A \equiv U - TS$$

$$C_V \equiv \left(\frac{dU}{dT}\right)_V = T\left(\frac{dS}{dT}\right)_V \qquad C_P \equiv \left(\frac{dH}{dT}\right)_P = T\left(\frac{dS}{dT}\right)_P$$

$$\wp_m \propto e^{-\frac{U_m}{k_B T}}$$

$$\wp(state) \propto \exp\left[-\frac{G(state)}{RT}\right]$$

$$\Delta G(T) = \Delta H_0\left(1 - \frac{T}{T_0}\right) + \Delta C_p\left[T - T_0 - T\ln\left(\frac{T}{T_0}\right)\right] \quad \text{(constant } C_p \text{ model)}$$

Chemical kinetics

$$k = k_0 e^{-\frac{\Delta G^{\ddagger}}{RT}}$$

$$\Delta G_{rxn} = \Delta G^{\circ}_{rxn} + RT\ln\frac{[B]}{[A]}$$

$$K_{eq} \equiv \exp\left(-\frac{\Delta G^{\circ}_{rxn}}{RT}\right)$$

$$K_{eq} = \frac{k_f}{k_r}$$

Protein folding

$$\frac{[F]}{[U]} = K = e^{-\frac{\Delta G^0_{\text{fold}}}{RT}}$$

$$[F] = \frac{k_f\left[1 - e^{-(k_f + k_u)t}\right]}{k_f + k_u}[U]_0$$

Ligand binding

$$\frac{[C]}{[P][L]} = K_A = \frac{1}{K_D} = \exp\left(-\frac{\Delta G^0_{\text{bind}}}{RT}\right)$$

$$\ln\frac{K_D(T_2)}{K_D(T_1)} = \frac{\Delta H(T_1)}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) + \frac{\Delta C_P}{R}\left[1 - \frac{T_1}{T_2} - \ln\left(\frac{T_2}{T_1}\right)\right] \quad \text{(constant } C_p \text{ model)}$$

$$\frac{[P]}{[P]_0} = \frac{1}{1 + K_{eq}[L]^n} \quad \text{(Hill equation)}$$

Enzyme kinetics

$$\frac{d[P]}{dt} = v = \frac{v_{\max}[S]}{[S] + K_M} \qquad v_{\max} \equiv k_2[E]_0 \qquad K_M \equiv \frac{k_{-1} + k_2}{k_1} \qquad \text{(Michaelis-Menten)}$$

mechanism	$\boldsymbol{v_{\text{max,app}}}$	$\boldsymbol{K_{M,\text{app}}}$	**special cases**
competitive inhibition	$v_{\max}$	$K_M\left(1 + \frac{[I]}{K_I}\right)$	*product inhibition*: v decreases with time
non-competitive inhibition	$v_{\max}\left(1 + \frac{[I]}{K_I'}\right)^{-1}$	$K_M\left(1 + \frac{[I]}{K_I'}\right)^{-1}$	*substrate inhibition*: v decreases more than expected with increasing $[S]$
mixed inhibition	$v_{\max}\left(1 + \frac{[I]}{K_I'}\right)^{-1}$	$K_M\left(1 + \frac{[I]}{K_I}\right)\left(1 + \frac{[I]}{K_I'}\right)^{-1}$	
pH-sensitive	$v_{\max}$	$K_{M,\text{app}} \equiv K_M\left(1 + \frac{K_3}{[H^+]} + \frac{[H^+]}{K_4}\right)$	

Membranes

$$[M]_0 = [M]\left[1 + \left(\frac{2[M]}{c^*}\right)^{n-1}\right] \qquad K_{eq} = \frac{1}{n}\left(\frac{2}{c^*}\right)^{n-1} \quad \text{(critical micelle concentration)}$$

$$\Pi = RT\Delta c \qquad \text{(osmotic pressure)}$$

$$\Delta V = -\frac{k_B T}{qe}\ln\left(\frac{c_i}{c_e}\right) \qquad \text{(Nernst equation)}$$

$$\approx \mp(60\ mV)\log_{10}\left(\frac{c_i}{c_e}\right) \quad \text{at } T = 300\ K \text{ for } \pm 1 \text{ charged ions}$$

Transport

$$J = P(c_1 - c_2) \qquad P = \frac{DH}{l}$$

$$D = \frac{k_B T}{6\pi\mu R} \qquad \text{(Stokes-Einstein)}$$

$$\langle r^2\rangle = 6Dt \qquad \text{(mean squared displacement)}$$

$$[P]_1 = \frac{v_{in}}{k_1}\left(1 - e^{-k_1 t}\right) \qquad [P]_2 = \frac{v_{in}}{k_2}\left(1 + \frac{k_1 e^{-k_2 t} - k_2 e^{-k_1 t}}{k_2 - k_1}\right) \qquad \text{(two-compartment model)}$$