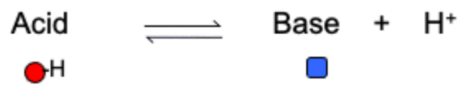
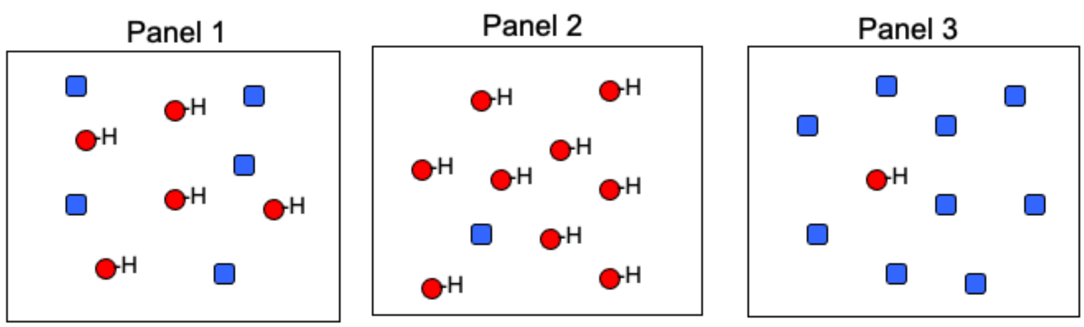
Quantitative Biology and Biophysics
Examination - Thermodynamics and Simulation

April 10, 2022
Instructor: Vincent J Hilser




1. For the above equilibrium between the Acid (Red) and Base (Blue) forms of the molecule, match the statement with the appropriate panel.

a) Panel 1: pH > pKa;  Panel 2:  pH = pKa;  Panel 3: pH < pKa.
b) Panel 1: pH < pKa;  Panel 2:  pH = pKa;  Panel 3: pH > pKa.
c) Panel 1: pH = pKa;  Panel 2:  pH > pKa;  Panel 3: pH < pKa.
d) Panel 1: pH = pKa;  Panel 2:  pH < pKa;  Panel 3: pH > pKa.
e) Panel 1: pH > pKa;  Panel 2:  pH < pKa;  Panel 3: pH = pKa.

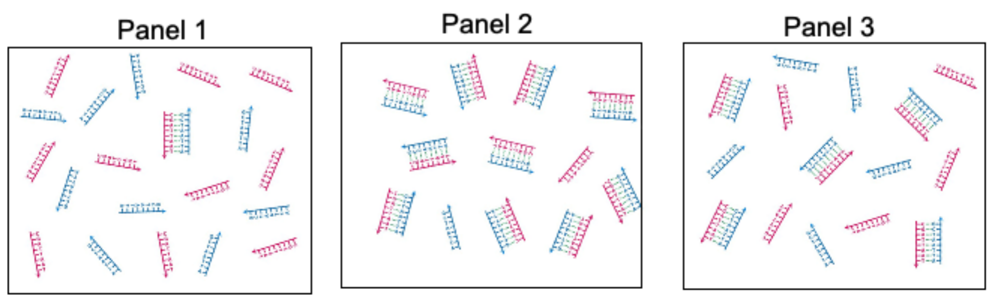


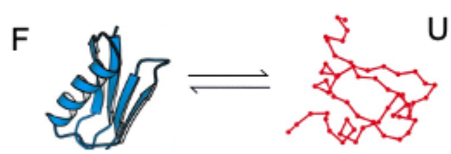

2. If the pKa for this reaction is 8, what is the pH in Panel 2

a) pH = 10
b) pH = 9
c) pH = 8
d) pH = 7
e) pH = 6


3. For the above equilibrium between the bound (B) and free (F) forms of DNA, match the statement about $\Delta G$ (= $G_B - G_F$) with the correct panel ?

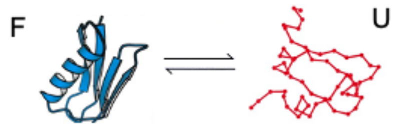
a) Panel 1: $\Delta G < 0$; Panel 2: $\Delta G > 0$; Panel 3: $\Delta G = 0$.
b) Panel 1: $\Delta G > 0$; Panel 2: $\Delta G < 0$; Panel 3: $\Delta G = 0$.
c) Panel 1: $\Delta G < 0$; Panel 2: $\Delta G = 0$; Panel 3: $\Delta G > 0$.
d) Panel 1: $\Delta G > 0$; Panel 2: $\Delta G = 0$; Panel 3: $\Delta G < 0$.
e) Panel 1: $\Delta G = 0$; Panel 2: $\Delta G > 0$; Panel 3: $\Delta G < 0$.



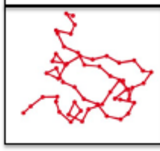

4. For the above equilibrium, what expression is true?

a) $K=e^{-\Delta S/RT}$.
b) $P_u=K_u/Q$.
c) $Q= \Sigma K$
d) $P_u= Q/K_u$
e) (b) and (c)



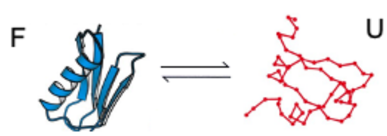

5. For the two-state transition above, match the expressions with the corresponding letters in the table.

i) 1
ii) $e^{-\Delta Gu/RT}/Q$
iii) $1/Q$
iv) 0
v) $e^{-\Delta Gu/RT}$
vi) $\Delta G_u$
vii) $1 + e^{-\Delta Gu/RT}$

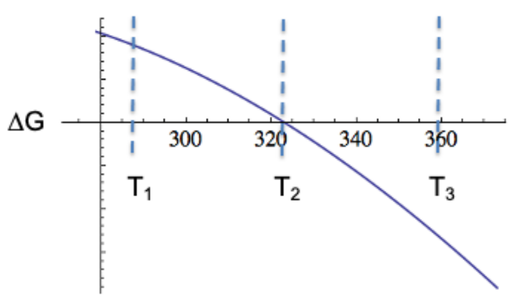
| | $\Delta G$ | Stat. Wt. | Probability |
|---|---|---|---|
|  | A | C | E |
|  | B | D | F |

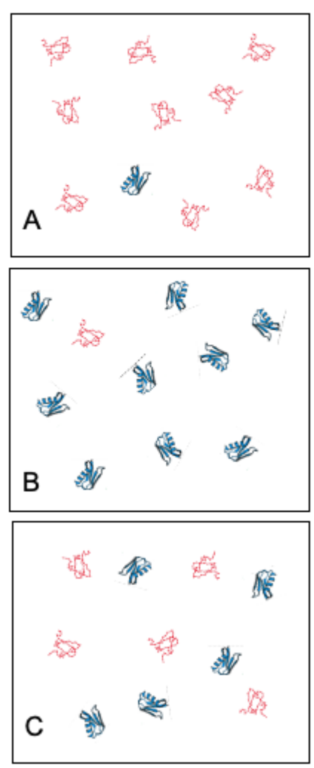
$Q = G$

a) A is (iv); B is (ii); C is (i); D is (vi); E is (vii), F is (iii); G is (v)
b) A is (i); B is (v); C is (iv); D is (vi); E is (iii), F is (ii); G is (vii)
c) A is (vi); B is (iv); C is (v); D is (i); E is (ii), F is (iii); G is (iv)
d) A is (iv); B is (vi); C is (i); D is (v); E is (iii), F is (ii); G is (vii)
e) A is (v); B is (ii); C is (i); D is (vi); E is (iii), F is (vii); G is (iv)

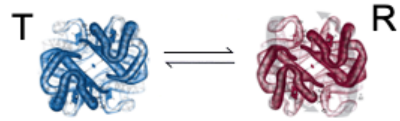



6. For the above equilibrium between the folded (F) and unfolded (U) forms of the protein where $\Delta G$ (= $G_U - G_F$), match the temperature with the panel that most closely captures the stability ?



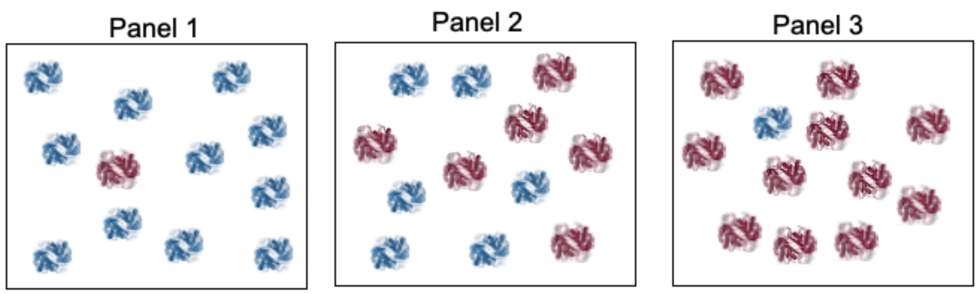



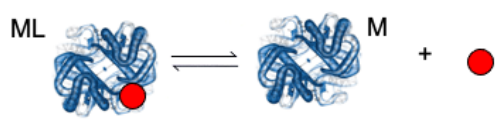

a) $T_1$ is C, $T_2$ is A, $T_3$ is B.
b) $T_1$ is B, $T_2$ is C, $T_3$ is A.
c) $T_1$ is A, $T_2$ is C, $T_3$ is B.
d) $T_1$ is C, $T_2$ is B, $T_3$ is A.
e) $T_1$ is B, $T_2$ is A, $T_3$ is C.




7. The hypothetical protein above has two states that are in equilibrium, T (Blue) and R (Red). Both T and R bind protons (H+) but the T state binds with higher affinity. At pH 7, $\Delta G^o$ ($G^o_R$-$G^o_T$) =0 (Panel 2). What statement best describes the effect of lowering the pH of the solution on the T to R equilibrium?

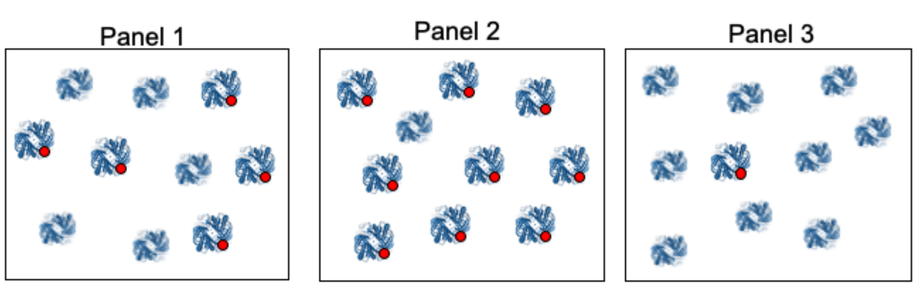
a) R will be stabilized (Panel 3).
b) T will be destabilized (Panel 3).
c) R will be destabilized (Panel 2).
d) T will be stabilized (Panel 1)
e) No change

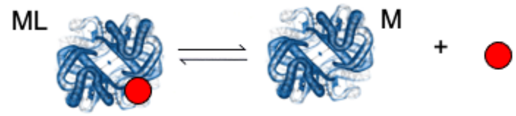



8. For the above equilibrium between the bound (ML) and free (M) forms of the molecule, match the statement with the appropriate panel.

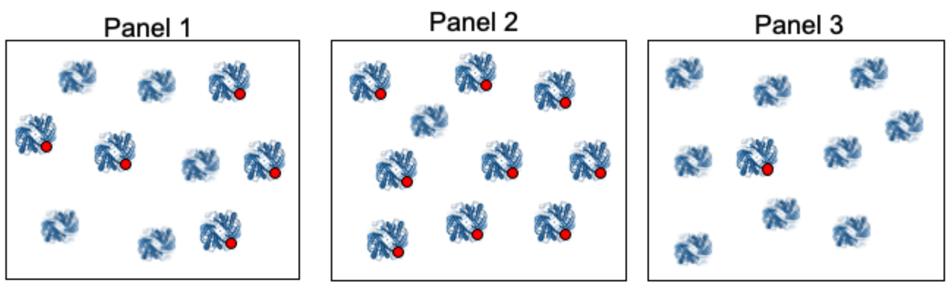
a) Panel 1: [L] < $K_d$; Panel 2: [L] > $K_d$; Panel 3: [L] = $K_d$.
b) Panel 1: [L] = $K_d$; Panel 2: [L] > $K_d$; Panel 3: [L] < $K_d$.
c) Panel 1: [L] > $K_d$; Panel 2: [L] = $K_d$; Panel 3: [L] < $K_d$.
d) Panel 1: [L] = $K_d$; Panel 2: [L] < $K_d$; Panel 3: [L] > $K_d$.
e) Panel 1: [L] > $K_d$; Panel 2: [L] > $K_d$; Panel 3: [L] = $K_d$.

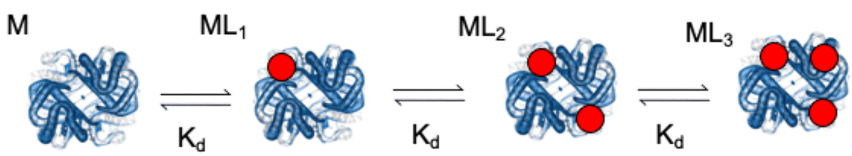





9. If the $K_d = 10^{-4}$ M, what is the concentration of [L] in Panel 3?

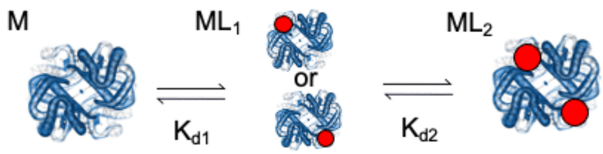
a) [L] = $10^{-7}$ M
b) [L] = $10^{-6}$ M
c) [L] = $10^{-5}$ M
d) [L] = $10^{-4}$ M
e) [L] = $10^{-3}$ M



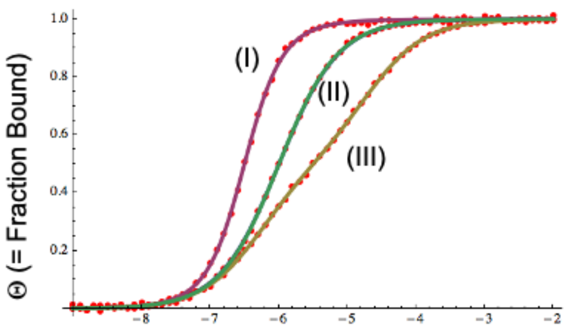

10. For the above case of a protein with three independent binding sites, what is the partition function.

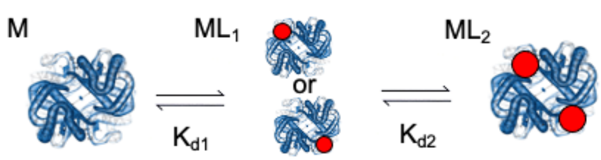
a) $Q = 1 + 3[L]/K_d + 3[L]^2/K_d^2 + [L]^3/K_d^3$
b) $Q = (1 + [L]/K_d)^3$
c) $Q = Q = 1 + 3[L]/K_d + 3[L]^2/K_d^2 + [L]^3/K_d^3$
d) (a) and (b)
e) (b) and (c)

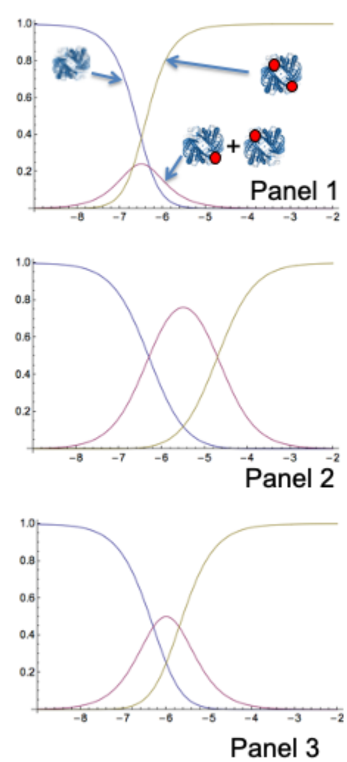



11. For the above case of a protein with two binding sites, match the statement about the relationship between $K_{d1}$ and $K_{d2}$ and the curve showing fraction bound as a function of Log[L].

a) (I) $K_{d2} < K_{d1}$ (II) $K_{d2} > K_{d1}$ (III) $K_{d2} = K_{d1}$
b) (I) $K_{d2} > K_{d1}$ (II) $K_{d2} < K_{d1}$ (III) $K_{d2} = K_{d1}$
c) (I) $K_{d2} > K_{d1}$ (II) $K_{d2} = K_{d1}$ (III) $K_{d2} < K_{d1}$
d) (I) $K_{d2} < K_{d1}$ (II) $K_{d2} > K_{d1}$ (III) $K_{d2} = K_{d1}$
e) (I) $K_{d2} < K_{d1}$ (II) $K_{d2} = K_{d1}$ (III) $K_{d2} > K_{d1}$

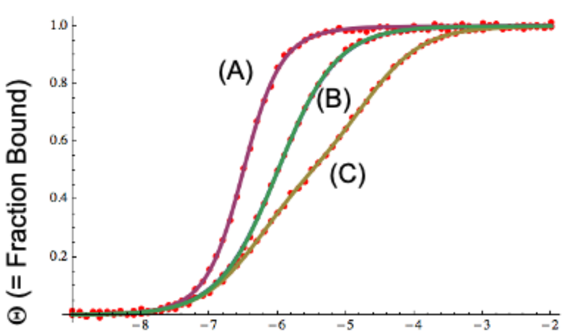


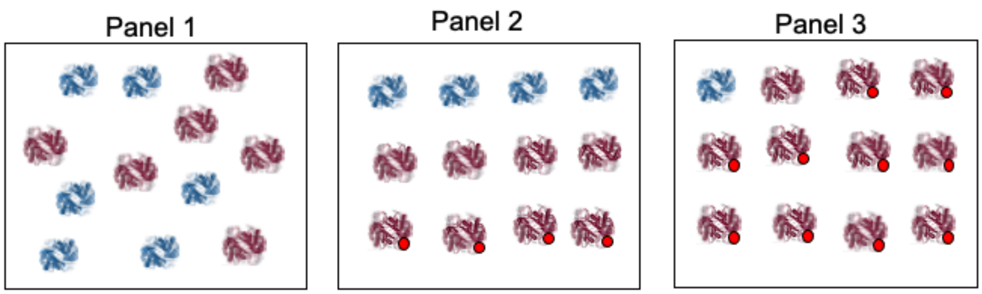

12. Which statement(s) about the cooperativity of the processes is true.

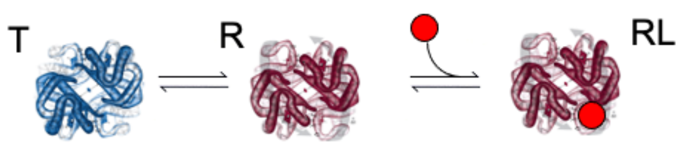
a) Panel 1 (curve C) shows positive cooperativity.
b) Panel 2 (curve A) shows positive cooperativity.
c) Panel 3 (curve B) shows no cooperativity.
d) (a) and (c)
e) None




13. The hypothetical protein above has two states that are in equilibrium, T (Blue) and R (Red), where only the R state can bind a ligand (L). In the absence of ligand the intrinsic equilibrium $\Delta G^o$ ($G^o{}_R - G^o{}_T$) = 0 (Panel 1). If the ligand binds to the R-state with a $K_d = 10^{-9}$, what are the ligand concentrations in panels 2 and 3?

a) Panel 2: [L] = $10^{-6}$ M; Panel 3: [L] = $10^{-7}$ M;
b) Panel 2: [L] = $10^{-9}$ M; Panel 3: [L] = $10^{-8}$ M;
c) Panel 2: [L] = $10^{-8}$ M; Panel 3: [L] = $10^{-10}$ M;
d) Panel 2: [L] = $10^{-10}$ M; Panel 3: [L] = $10^{-8}$ M;




14. The hypothetical protein above has two states that are in equilibrium, T (Blue) and R (Red), where only the R state can bind a ligand (L). In the absence of ligand the T state is favored by a ratio of 10:1 (Panel 1). If the ligand binds to the R-state with a $K_d = 10^{-9}$, what are the ligand concentrations in panels 2 and 3?

a) Panel 2: [L] = $10^{-6}$ M; Panel 3: [L] = $10^{-7}$ M;
b) Panel 2: [L] = $10^{-9}$ M; Panel 3: [L] = $10^{-8}$ M;
c) Panel 2: [L] = $10^{-8}$ M; Panel 3: [L] = $10^{-10}$ M;
d) Panel 2: [L] = $10^{-10}$ M; Panel 3: [L] = $10^{-8}$ M;