

Homework Assignment 5 – Hydrogen Exchange

DUE in class, Thursday, October 19th

1. Hydrogen exchange experiments were done on a protein and the rates of hydrogen exchange in various concentrations of guanidinium chloride were determined for two residues, *A* and *B*. The k_{ex} data are listed below:

Residue *A*

[GdmCl] (<i>M</i>)	k_{ex} (s^{-1})
0.5	4.412×10^{-6}
1.0	1.027×10^{-5}
1.5	4.696×10^{-5}
2.0	1.163×10^{-3}
2.5	3.410×10^{-2}

Residue *B*

[GdmCl] (<i>M</i>)	k_{ex} (s^{-1})
0.5	4.613×10^{-8}
1.0	1.353×10^{-6}
1.5	3.966×10^{-5}
2.0	1.163×10^{-3}
2.5	3.410×10^{-2}

Assume that the conditions were such that k_u , k_f are much greater than k_{ch} , that the k_{ch} for both residues is 1.0 s^{-1} and that $RT = 0.592 \text{ kcal mol}^{-1}$ at the experimental temperature.

Estimate the unfolding free energy for both residues at zero guanidinium Cl concentration.

- A. Email pat.fleming@jhu.edu a plot of the extrapolated unfolding free energies for residues *A* and *B* versus guanidinium Cl concentration. You may use Xmgrace or any other plotting program. The extrapolation to zero guanidinium Cl concentration can be done using a poly fit function (approximate intercept is fine). Put both data sets on the same plot; show the data as symbols; indicate your estimates for the unfolding free energy of each residue.
- B. In the body of the email provide a short answer to the following question: Which residue is most likely to be in an unfolded region of the protein at zero concentration guanidinium Cl? Explain how you arrived at your answer.