

General concepts

- 1) The _____ the K_d , the HIGHER the binding affinity.
- 2) The _____ the K_d , the LOWER the binding affinity.
- 3) When a reaction is at equilibrium, what is staying constant?

Some examples

- 1) Protein P binds to ligand L, which is the first step in an arbitrary disease process. This interaction occurs with a K_d of 10 nM. In order to stop the disease process, we have developed a small molecule drug that we hope will disrupt ligand L to protein P interactions by binding to protein P itself. We have measured the amount of complex formation our drug achieves with protein P and obtained the following titration curve:

Given what you know about how K_d 's relate to binding affinity, which will bind better with Protein P, our drug or ligand L?

Is our drug likely to be effective in competing with ligand L?

- 2) We are given some values of ΔG and ΔH and we are asked to write a MATLAB function file that uses Gibb's free energy equation ($\Delta G = \Delta H - T\Delta S$) to calculate ΔS for each set of ΔG and ΔH 's.

What are the inputs to this function file? What form are the inputs in?

What are the outputs to this function file? What forms are they in?

Can we use Gibb's free energy equation as is ($\Delta G = \Delta H - T\Delta S$)?

Now let's write a mock function file:

How do we save this function file?