Relating back to $\Delta G°$:

Think about the binding reaction between a macromolecule M and some ligand X.

$$M + X \rightleftharpoons MX$$
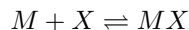
The free energy of this interaction depends on the intrinsic interaction energy between these molecules (under standard conditions: all components at 1 M, standard temperature and pressure) and the concentrations of all species in solution. We can write:

$$\Delta G([M], [X], [MX]) = \Delta G° + RTln\left(\frac{[M][X]}{[MX]}\right)$$

At $[MX] = [M]$, $\Delta G = 0$. $[M]$ and $[MX]$ cancel, giving:

$$0 = \Delta G° + RTln\left([X]_{[MX]=[M]}\right)$$

$$\Delta G° = -RTln([X]_{[MX]=[M]})$$

This special concentration $[X]_{[MX]=[M]}$—the concentration of X at which M is half-saturated—is defined as the K_D:

$$[X]_{[MX]=[M]} = K_D$$

$$\Delta G° = -RTln(K_D)$$

$$\Delta G = -RTln(K_D) + RTln\left(\frac{[M][X]}{[MX]}\right)$$

Full binding equilibrium:

We're often interested in the fractional saturation of M at a given concentration of X. This is given by Θ, defined as:

$$\Theta = \frac{[MX]}{[M] + [MX]}$$

We'd like to write an expression for Θ in terms of K_D and things we can manipulate experimentally: $[M]_{tot}$ and $[X]_{tot}$.

If we let the system come to equilibrium, $\Delta G \equiv 0$:

$$0 = -RTln(K_D) + RTln\left(\frac{[M][X]}{[MX]}\right)$$

$$RTln(K_D) = RTln\left(\frac{[M][X]}{[MX]}\right)$$

$$K_D = \frac{[M][X]}{[MX]}$$

We also need to establish mass-action:

$$[M]_{tot} = [M] + [MX]$$

$$[X]_{tot} = [X] + [MX]$$

Our problem is that we can experimentally alter $[M]_{tot}$ and $[X]_{tot}$, but have no access to $[X]$, $[M]$, or $[MX]$. We're going to do some algebra to write out a relationship for Θ that does not involve terms we can't access. First, rearrange:

$$[M] = [M]_{tot} - [MX]$$

$$[X] = [M]_{tot} - [MX]$$

Substitute and rearrange again:

$$K_D = \frac{([M]_{tot} - [MX])([X]_{tot} - [MX])}{[MX]}$$

$$K_D = \frac{[M]_{tot}[X]_{tot} - [X]_{tot}[MX] - [M]_{tot}[MX] + [MX]^2}{[MX]}$$

$$K_D[MX] = [M]_{tot}[X]_{tot} - [X]_{tot}[MX] - [M]_{tot}[MX] + [MX]^2$$

$$0 = [M]_{tot}[X]_{tot} - [X]_{tot}[MX] - [M]_{tot}[MX] - K_D[MX] + [MX]^2$$

$$0 = [M]_{tot}[X]_{tot} - ([X]_{tot} + [M]_{tot} + K_D)[MX] + [MX]^2$$

Find the positive root of $[MX]$ using the quadratic formula:

$$[MX] = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$a = 1$$

$$b = -([X]_{tot} + [M]_{tot} + K_D)$$

$$c = [M]_{tot}[X]_{tot}$$

$$[MX] = \frac{[X]_{tot} + [M]_{tot} + K_D - \sqrt{([X]_{tot} + [M]_{tot} + K_D)^2 - 4[M]_{tot}[X]_{tot}}}{2}$$

Finally, find the fractional saturation:

$$\Theta = \frac{[MX]}{[M]_{tot}}$$

$$\Theta = \frac{[X]_{tot} + [M]_{tot} + K_D - \sqrt{([X]_{tot} + [M]_{tot} + K_D)^2 - 4[M]_{tot}[X]_{tot}}}{2[M]_{tot}}$$

This relationship is ugly, but correct.

Limiting case of low $[M]_{tot}$:

If $[M]_{tot} \ll K_D$, binding will never deplete $[X]_{tot}$ appreciably (meaning $[X] \approx [X]_{tot}$). This simplifies things.

$$K_D = \frac{[M][X]}{[MX]}$$

$$K_D \approx \frac{([M]_{tot} - [MX])[X]_{tot}}{[MX]}$$

$$K_D[MX] = ([M]_{tot} - [MX])[X]_{tot}$$

$$K_D[MX] = [M]_{tot}[X]_{tot} - [MX][X]_{tot}$$

$$K_D[MX] + [X]_{tot}[MX] = [M]_{tot}[X]_{tot}$$

$$[MX](K_D + [X]_{tot}) = [M]_{tot}[X]_{tot}$$

$$[MX] = \frac{[M]_{tot}[X]_{tot}}{K_D + [X]_{tot}}$$

$$\Theta = \frac{[MX]}{[M]_{tot}} = \frac{[M]_{tot}[X]_{tot}}{[M]_{tot}(K_D + [X]_{tot})}$$

$$\Theta = \frac{[X]_{tot}}{K_D + [X]_{tot}}$$