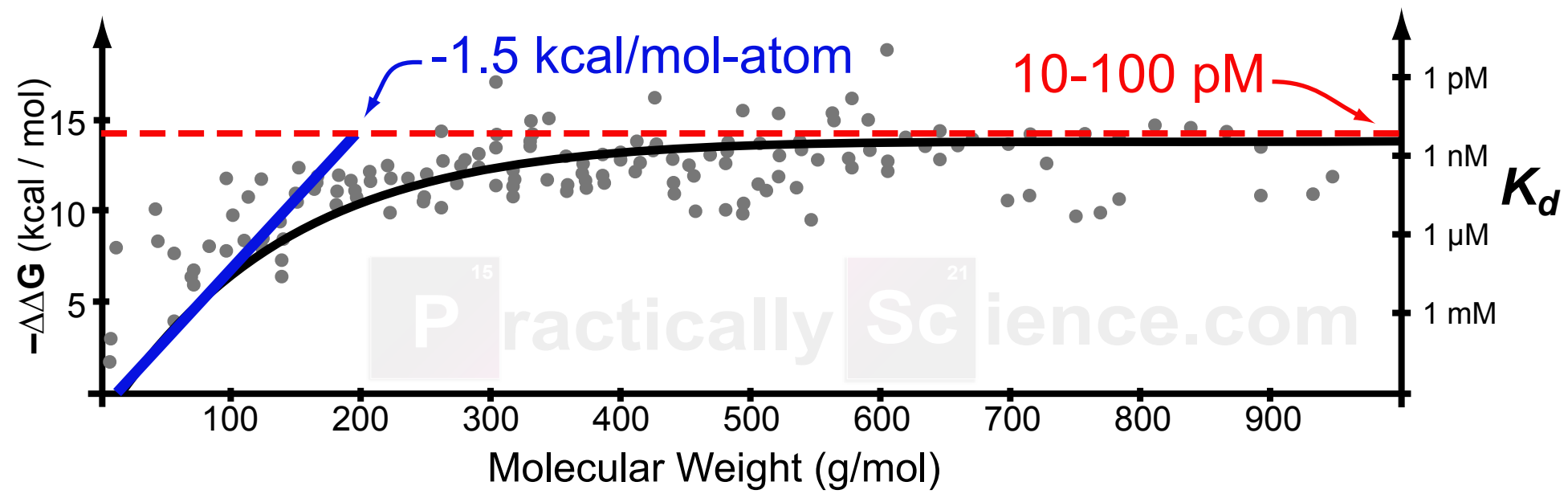


The Maximum Affinity of Small Molecules Ligands



Linear Regime 1: near max ΔG /atom

Maximum Van Der Waals

$\Delta H \approx$
-1 kcal / mol-atom

Maximum hydrophobic effect

$-T\Delta S \approx$
-1 kcal / mol-atom

+

Linear Regime 2: enthalpy-entropy comp

\uparrow enthalpic binding (*tighter spring*)
 =
 \uparrow entropic penalty (*less vibration*)