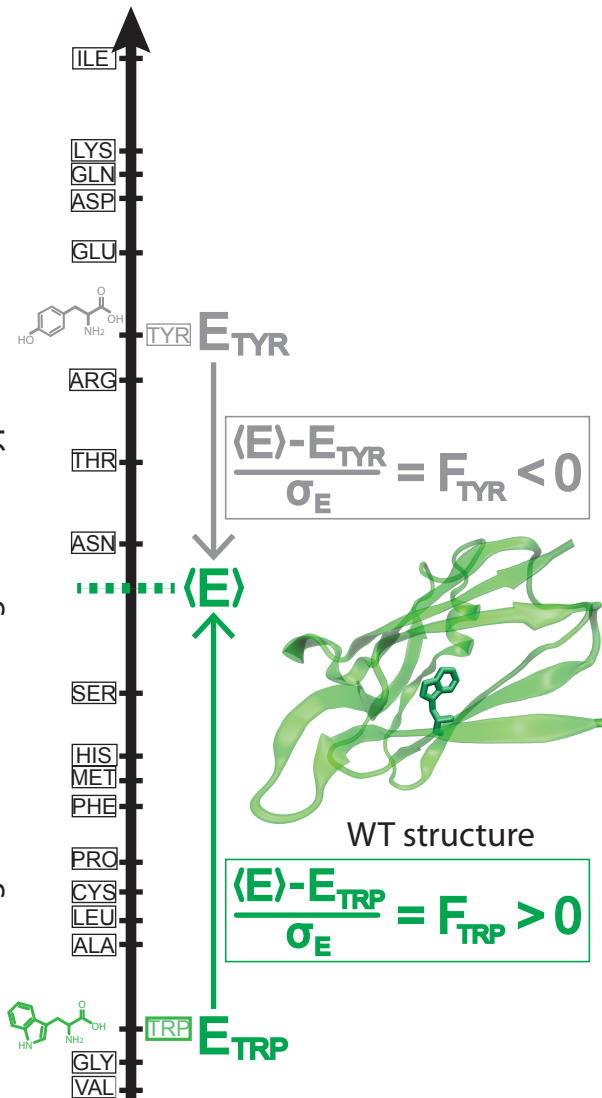


Measuring perturbation  
with naive calculation

$$F_{\text{TYR}} - F_{\text{TRP}} = \tilde{\Delta F} < 0$$

Energies calculated using the wild-type structure



Measuring perturbation  
with secondary calculation

$$F'_{\text{TYR}} - F_{\text{TRP}} = \Delta F < 0$$

