

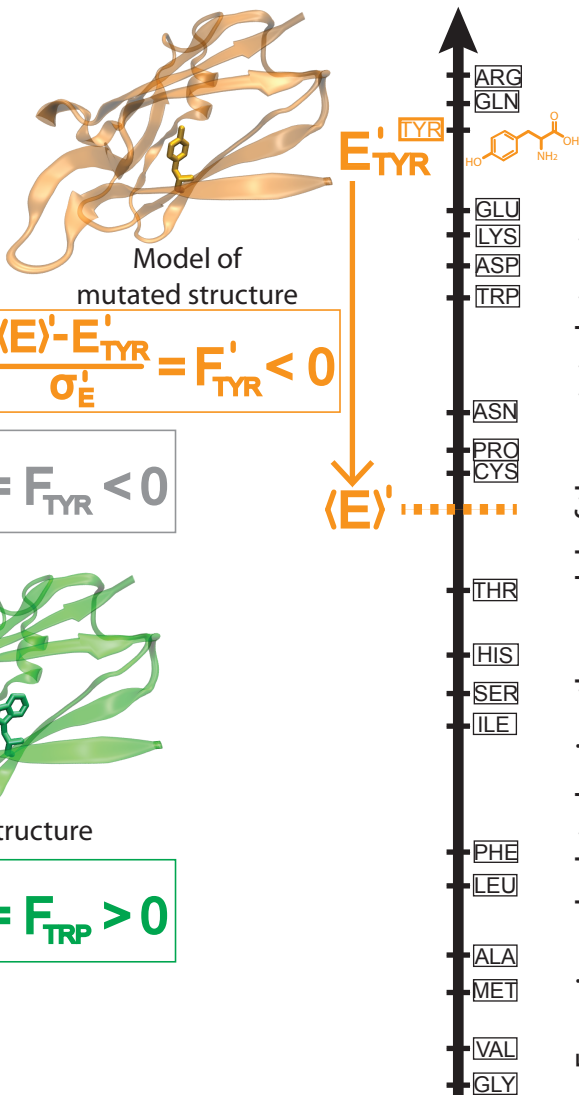
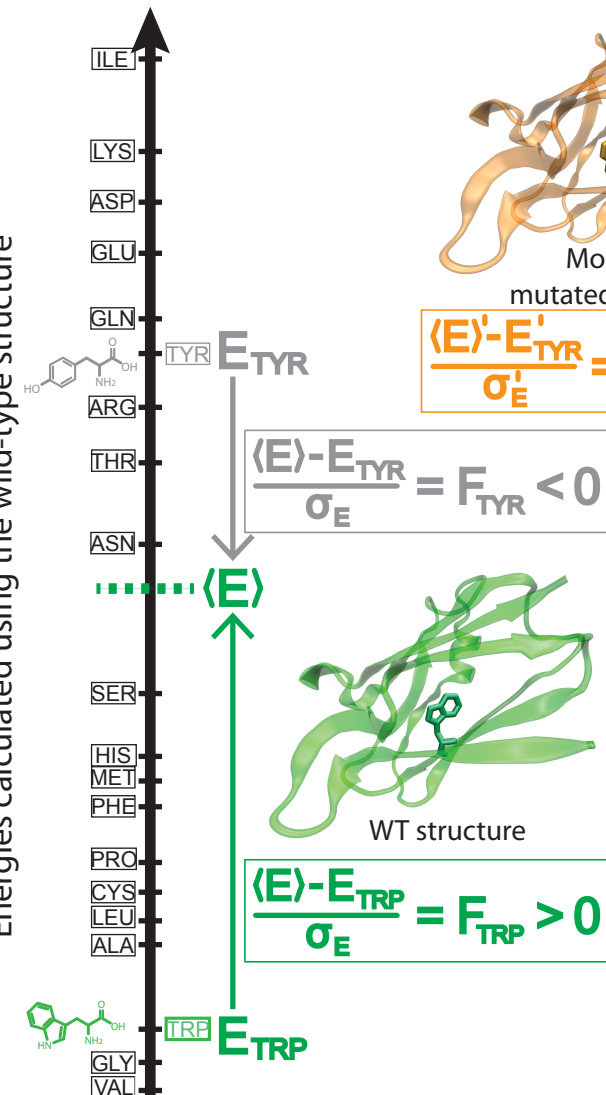
Measuring perturbation
with naive calculation

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

Measuring perturbation
with secondary calculation

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

Energies calculated using the wild-type structure



Energies calculated using the model of the mutated structure