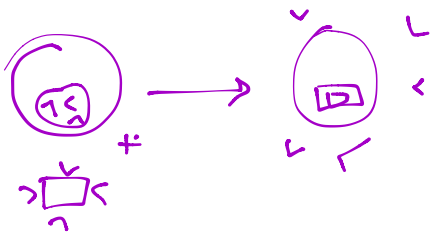
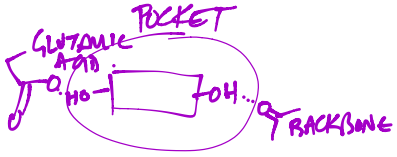
ESTRADIOL

TESTOSTERONE

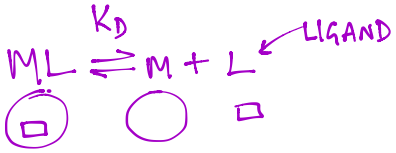
RECEPTOR





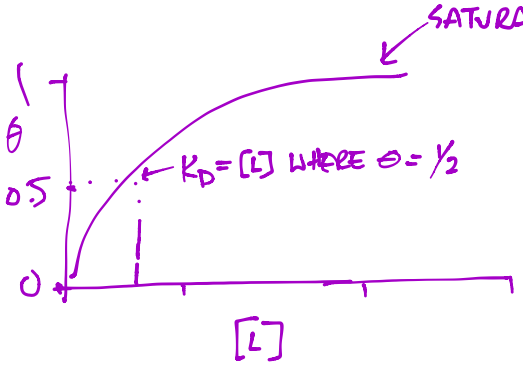
		HPHOBE/H_2O	HBOND		HPHOBE/H_2O	HBOND
UNBOUND STEROID	E	LOTS	YES (H_2O)	T	LOTS	YES (H_2O)
	R	LOTS	YES (H_2O)	R	LOTS	YES (H_2O)
BOUND STEROID	E	LESS	YES (R)	T	LESS	LESS
	R	LESS	YES (E)	R	LESS	LESS
NET BINDING CONTRIBUTION		FAVORABLE	∅		FAVORABLE	UNFAVORABLE

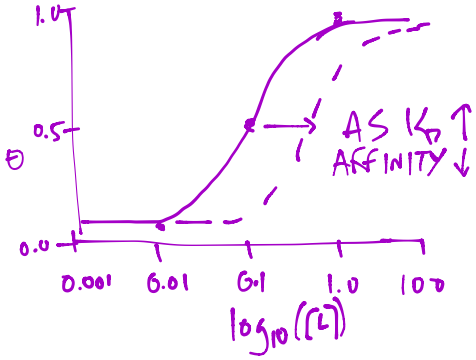
SPECIFICITY BY EXCLUDING BAD POLAR CONTACTS.



$$K_D = \frac{[M][L]}{[ML]} \rightarrow [M] = \frac{K_D[ML]}{[L]}$$

$$\theta = \frac{[ML]}{[M]+[ML]} = \frac{[ML]}{\frac{K_D[ML]}{[L]}+[ML]} = \frac{1}{1+K_D/[L]}$$





DOES H-BOND EXPLAIN?

$\Delta G_{EST} = -RT\ln(K_D)$

$K_{D,EST} = 1E\text{-}10\ M$

$K_{D,TES} = 1E\text{-}4\ M$

$= -0.0083 \cdot 300 \cdot \ln(1E-10)$

$= +57$ kJ/mol

$\Delta G_{TES} = +23$ kJ/mol

ENERGY TO DISSOCIATE

$\Delta\Delta G = 34$ kJ/mol ~ 20 kJ/mol ENERGY H BOND.