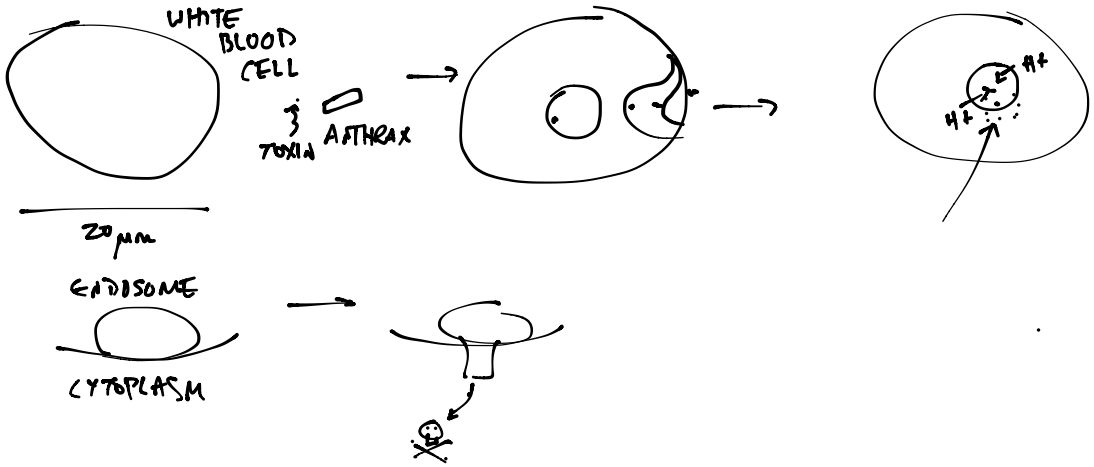
SMALL MOLECULES, BIG EFFECTS:

AN INSPIRATIONAL TALE



ON SCREEN QUESTIONS:

IF WE'RE GOING TO ANSWER QUESTION WELL, WE NEED SOME WAY TO TREAT $[H^+]$

START WITH GOALS
QUIZ ABOUT pH
COMPLAIN ABOUT UNITS... ~ CARLSBERG

$[H^+] \rightarrow pH \equiv -\log_{10}([H^+])$

$[H^+] = 10^{-pH}$

CARBOXYLIC ACID 

AMINE $R\text{-}NH_3^+ \rightleftharpoons R\text{-}NH_2 + H^+$

K_{ACID}

$\frac{[H^+][A^-]}{[HA]} \rightarrow [A^-]$

$\frac{[H^+][A^-]}{[HA]}$

HOW DO WE LINK pH TO K_a?

pH → K_a?

$K_a = \frac{[H^+][A^-]}{[HA]}$

$-\log_{10}(K_a) = -\log_{10}\left(\frac{[H^+][A^-]}{[HA]}\right)$

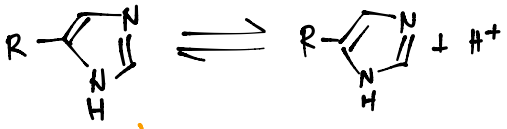
$pK_a = -\log_{10}[H^+] - \log_{10}\left(\frac{[A^-]}{[HA]}\right)$

$pK_a = pH - \log_{10}\left(\frac{[A^-]}{[HA]}\right)$

$pH = pK_a + \log\left(\frac{[A^-]}{[HA]}\right)$

NOT GOING TO TALK ABOUT BUFFERING ... GOING TO WORRY MORE ABOUT [A] VS. [HA].

HISTIDINE:



@ SOME pH, WHAT IS CHARGE ON HISTIDINE?

$\theta \equiv$ FRACTIONAL PROTONATION

$= \frac{[HA]}{[HA]+[A]} \in [0,1]$

$pH = pK_a + \log\left(\frac{[A]}{[HA]}\right)$

$pH - pK_a = \log\frac{[A]}{[HA]}$

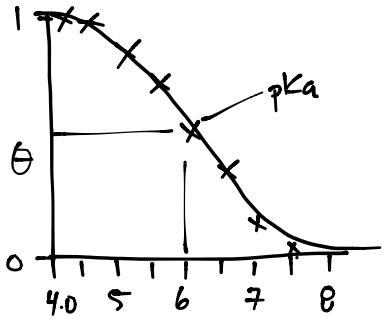
$10^{pH-pK_a} = \frac{[A]}{[HA]}$

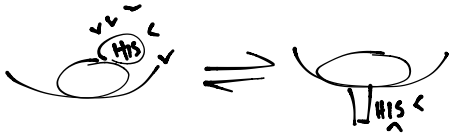
$[HA]10^{pH-pK_a} = [A]$

$\theta = \frac{[HA]}{[HA]+[HA]\cdot 10^{pH-pK_a}}$

$\theta = \frac{1}{1+10^{pH-pK_a}}$

pH	θ	ΔG_{TOX}
7.5	0.03	> 0
7.0	0.09	
6.5	0.24	
6.0	0.50	
5.5	0.76	
5.0	0.91	
4.5	0.97	< 0
4.0	0.99	





LE CHÂTELIER'S PRINCIPLE

$pH \sim \Delta G$

$RT\ln(10)(4.5-7.5) = -18\,kJ/mol$