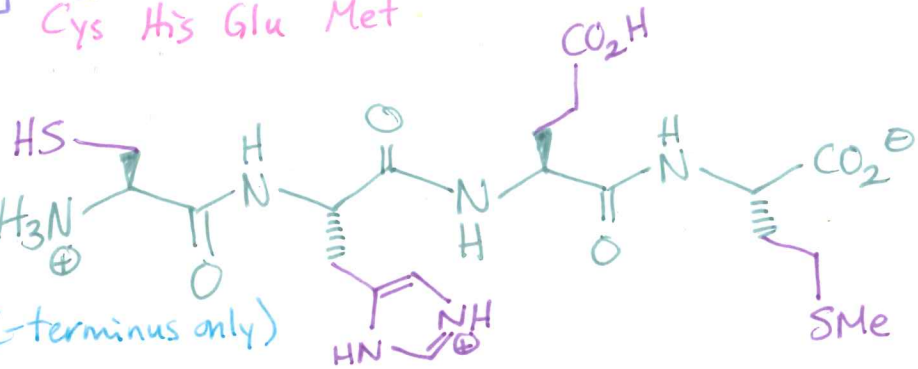
Lecture 6 HW Key

26.38 (a) C-H-E-M
Cys His Glu Met

pH 3

past pKa_1 Met
(effects C-terminus only)

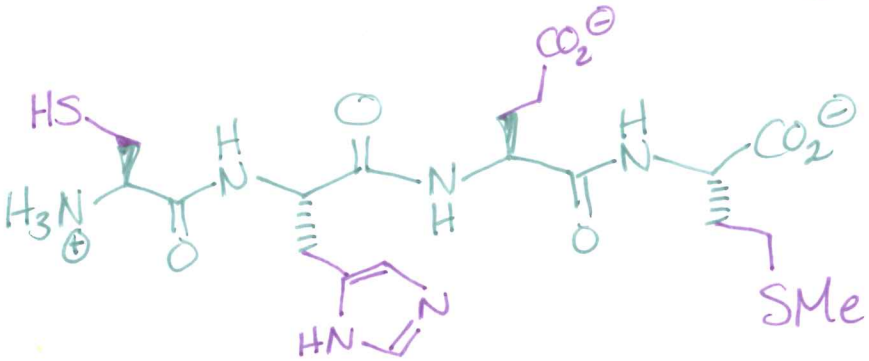


net charge +1

(in case you were curious, and you should be!)

pH 7.4

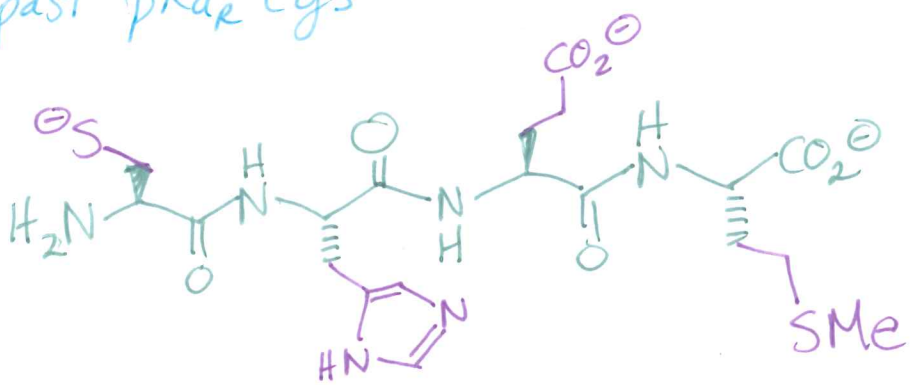
past pKa_R Glu
&
pKa_R His



net charge -1

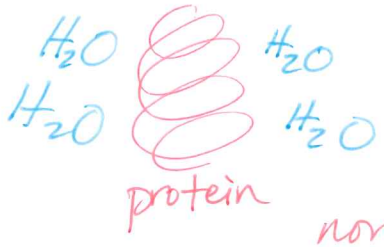
pH 10

past pKa_2 (effects N-terminus only; amide N-H's not acidic)
also past pKa_R Cys



net charge -3

26.44 Where is each aa found inside vs. outside of protein?



polar/charged aa side chains found on outside of protein (hydrophilic)

non-polar/noncharged aa side chains buried inside protein (hydrophobic)

(c) Phe & (a) Val - neutral side chain (hydrocarbon)
always inside protein, never charged

(b) Asp

pH 3
side chain polar, not charged
likely on outside of protein
could be inside

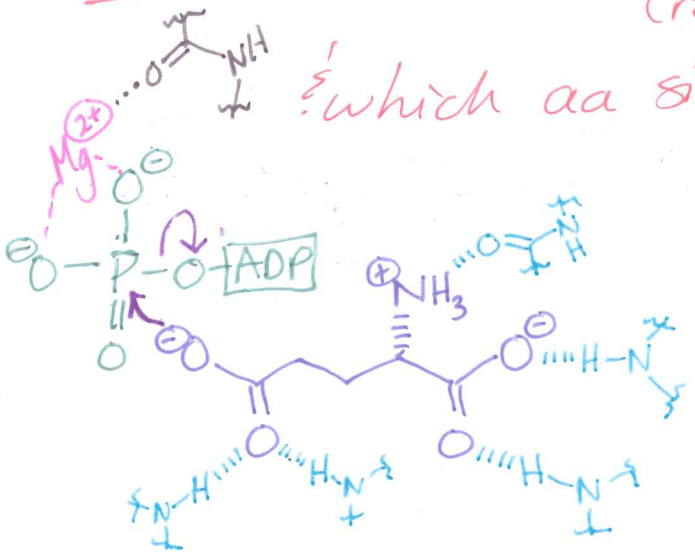
pH 7.4
side chain (charged)
more likely on outside of protein

pH 10
deprotonated

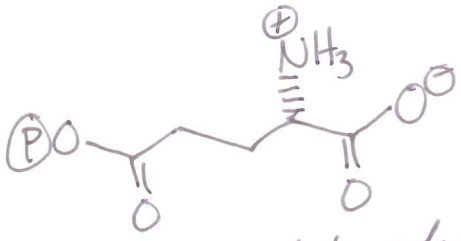
(c) Lys - side chain protonated (charged) @ pH 3, 7.4, & 10
found on outside of protein

Enzyme Active Site Design

Consider: how substrates & co-factors (reagents) are held in place & which aa side chains are appropriate acids & base

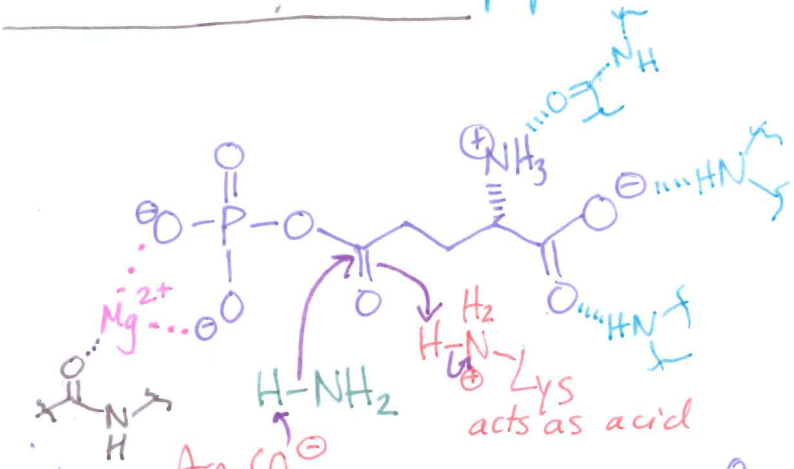


ATP ATP

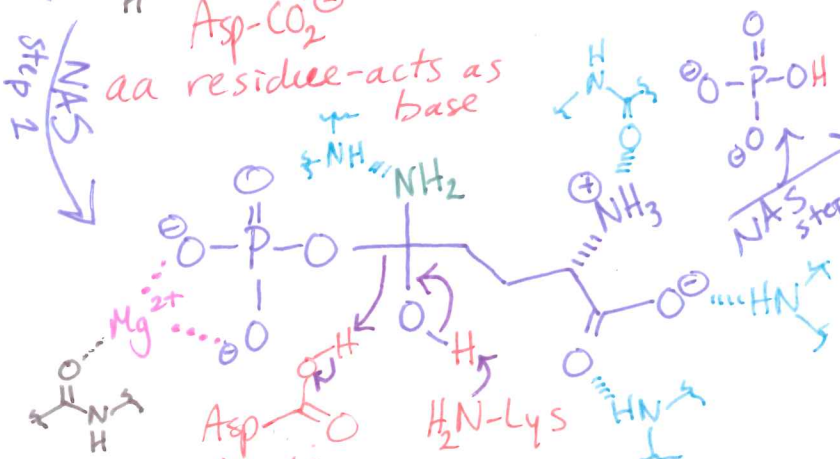


no need to show stabilization after rxn, unless it goes through another step...

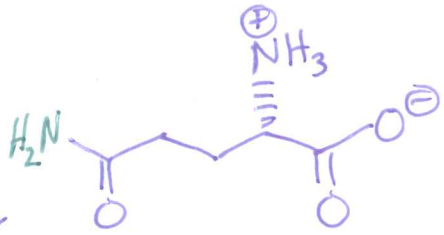
* H bonding to peptide backbone



NAS step 2



NAS step 2



* re-use aa's when possible *

Note: arrow-pushing is same as in L5 HW! Difference is defining $H^{\oplus}$ & :B as aa residues & adding stabilizing factors (H-bonding or metal)