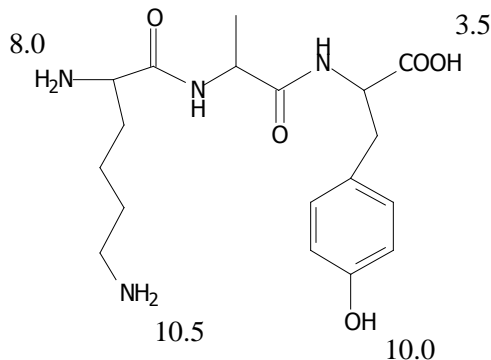


### Biochemistry Problem Set 3 - Due Monday October 1<sup>st</sup>

1. (20 points) Consider the following peptide derivative. The molecule is drawn with its functional groups in their neutral form. The  $pK_a$  for each of the ionizable groups are indicated.



- Draw the predominant forms of the aqueous ionic species at pH 2, 6, 9, and 12
  - Calculate the value of the pI of this peptide. Indicate the predominant ionic species at the pI of the molecule.
2. (30 points) The amino acid glycine is often used as the main ingredient of a buffer in biochemical experiments. The amino group of glycine, which has a  $pK_a$  of 9.6, can exist either in the protonated form ( $-NH_3^+$ ) or as the free base ( $-NH_2$ ) because of the reversible equilibrium:

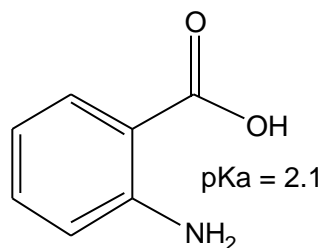
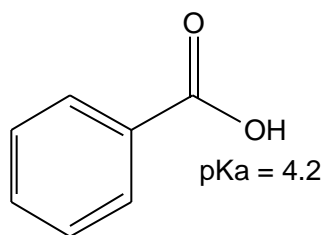


- In what pH range can glycine be used as an effective buffer due to its amino group?
  - In a 0.1 M solution of glycine at pH 9.0, what fraction of glycine has its amino group in the  $-NH_3^+$  form?
  - How much 5 M KOH must be added to 1.0 L of 0.1 M glycine at pH 9.0 to bring its pH to exactly 10.0?
  - In order to have 99% of the glycine in its  $-NH_3^+$  form, what must the numerical relation be between the pH of the solution and the  $pK_a$  of the amino group of glycine?
3. (20 points) You have a cation exchange resin in a column and plan to separate the following amino acid mixtures:

- i) A; E; R      ii) H; G; D      iii) K; E; W      iv) M; E; H

For each case, indicate how would you modify the pH in order to get the maximum separation of the amino acid mixtures, and the order in which the amino acids of the different mixtures would come out of the column.

4. (20 points) The pKa of the carboxylate group in the benzoic acid is approximately 4.2, while in *o*-amino benzoic acid it is 2.1



- i) Explain why the pKa of plain benzoic acid is higher than the pKa of *o*-amino benzoic acid.
  - ii) With what functional group would you replace the amine in order to increase the pKa of the carboxylate above the pKa of benzoic acid? Explain briefly.
5. (20 points) Calculate the approximate pIs of the following peptides, as well as their total charges at pH 1, 7, and 14. Show your work!
- i) Ala-Ala-Ala
  - ii) APVFGM
  - iii) Ala-Pro-Ala-Met-Glu
  - iv) IKGPNQEARS
6. (10 points) In the following molecules, which groups will be hydrogen bond donors and which ones hydrogen bond acceptors.

