BCHM 463 GSS - 09/12/2022

Acid Base Chemistry, Amino Acids, Protein Structure

(1.) For each of the polypeptide sequences below, give the sequence as one letter abbreviations.

a.)
$${}^{\dagger}H_2N \longrightarrow NH_2$$

$${}^{\dagger}H_3N \longrightarrow H$$

$${}^{\dagger}H_3N \longrightarrow H$$

c.) The charge of which peptide would be most affected by a shift in pH from 7.4 (as drawn) to a pH of 12? Explain.

Functional Group

pKa

Functional Group	рКа
Carboxyl-terminus	3.5
Amino-terminus	8.5
α-Carboxyl (free amino acid)	2
α-Amino (free amino acid)	9.5
Aspartate R group	3.9
Glutamate R group	4.2
Histidine R group	6
Cysteine R group	8.2
Tyrosine R group	10.0
Lysine R group	10.5
Arginine R group	12.5

(2.) Below is a structure for the dipeptide Glu-Cys. Draw a titration curve for this dipeptide, then determine the pI, given the pKa values as listed below. Make sure to label your axes!

Functional Group	pKa
Carboxyl-terminus	3.5
Amino-terminus	8.5
α-Carboxyl (free amino acid)	2
α-Amino (free amino acid)	9.5
Aspartate R group	3.9
Glutamate R group	4.2
Histidine R group	6
Cysteine R group	8.2
Tyrosine R group	10.0
Lysine R group	10.5
Arginine R group	12.5

(3.) Below is a structure for the polypeptide chain N' - CHEMISTRY - C'. Determine the pI of this chain. You do not need to draw a titration curve.

Functional Group	pKa
Carboxyl-terminus	3.5
Amino-terminus	8.5
α-Carboxyl (free amino acid)	2
α-Amino (free amino acid)	9.5
Aspartate R group	3.9
Glutamate R group	4.2
Histidine R group	6
Cysteine R group	8.2
Tyrosine R group	10.0
Lysine R group	10.5
Arginine R group	12.5

- (4.) Below is a table of common biological buffers and their pKa values.
- a.) In the research lab you are working at, you are asked to make 1L of buffer for a system at a pH of 8.0. You have several options for making this buffered system, as detailed below. Which of the choices would be the best? Explain why the other mixtures would not be optimal.

Choice	Buffer Material	рKа	Moles Conjugate Acid	Moles Conjugate Base
A	$\mathrm{H}_2\mathrm{CO}_3 \rightleftharpoons \mathrm{HCO}_3^{-2}$	6.77	9.5	2.5
В	Tris	8.1	10	0.5
C	MOPS	7.2	1.2	8.35
D	Glycylglycine	8.27	0.1	2

b.) Suppose you need to make three different solutions of MOPS buffer that each contain a total MOPS concentration (acid + conjugate base) of 0.5 M but are at different pH values. For each of the following pH values, what are the concentrations of the acid form of MOPS and the conjugate base form of MOPS?

i.)
$$pH = 5$$

ii.)
$$pH = 7$$

iii.)
$$pH = 10.5$$

c.) For the buffer chosen in part (a), would the buffer solution be more resistant to decreases or increases in the pH of the system? Explain why.

(5.) Suppose the polypeptide chain N' - GLSCRIQDEFECY	- C' spontaneously	forms an α -	helix in a
solution with a pH of 7.4.			

a.) Name at least 3 *different* intrahelical interactions between side chains in the polypeptide chain. Make sure to specify what amino acids are interacting, and what kind of interaction is present.

b.) If the pH is increased from 7.4 to 11, the secondary α -helical structure of this chain becomes distorted. Why might this be happening? Consider how different pH environments may affect intrahelical interactions of the polypeptide chain.

Functional Group	рКа
Carboxyl-terminus	3.5
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Histidine R group	6
Cysteine R group	8.2
Tyrosine R group	10.0
Lysine R group	10.5
Arginine R group	12.5