# Practice questions and explanations

#### BIOS 1006

#### Week 1

### Lecture 1: Fundamentals

### Functional groups

Question 1: Naming



#### Answers:

methyl, hydroxyl, thiol, carbonyl, carboxyl, amino, phosphate

#### Question 2: Roles of functional groups

- 1. Amino acids and proteins have amine groups & carboxyl groups.
- 2. Carbohydrates tend to have an abundance of hydroxyl groups and glycosidic linkages.
- 3. Lipids vary greatly in structure, but fatty acids typically have carboxyl groups.
- 4. Each nucleotide in a nucleic acid molecule has phosphodiester linkages.

## pH and pKa

#### Question 3: ICE tables and Henderson-Hasselbalch equation

You make a 0.2 M aqueous solution of propionic acid CH<sub>3</sub>CH<sub>2</sub>COOH by dissolving an appropriate amount of propionic acid in water. The pH of the resulting solution is 4.88. What is the pKa of propionic acid?

$$CH_3COOH \rightleftharpoons CH_3COO^- + H^+$$

Set up the ICE table:

|                      | [CH <sub>3</sub> COOH] | $[CH_3COO-]$ | $ [H^+] $ |
|----------------------|------------------------|--------------|-----------|
| Initial              | 0.2                    | О            | О         |
| Change               | -X                     | +x           | +x        |
| $\operatorname{End}$ | 0.2-x                  | +x           | +x        |

Given that the concentration of H<sup>+</sup> is equal to x, we can undo the logarithm to find [H<sup>+</sup>]:

$$pH = -\log[H^{+}]$$

$$4.88 = -\log[H^{+}]$$

$$[H^{+}] = 1.32 \times 10^{-5} M$$

Now plug this into the Henderson-Hasselbalch equation:

$$4.88 = pK_a + \log\left(\frac{1.32 \times 10^{-5}}{0.2 - 1.32 \times 10^{-5}}\right)$$

$$4.88 = pK_a + \log(6.6 \times 10^{-5})$$

$$4.88 = pK_a - 4.18$$

$$pK_a = 4.88 + 4.18$$

$$pK_a = \boxed{9.06}$$

## Lecture 2: Amino acids and peptides

Question 4: Amino acid chemical properties

Which amino acid side chains are ionizable? YECDHKR

Which amino acid has no chiral center? G

Which amino acids have hydrophobic (nonpolar) side chains? AVLIGMPFWY

Which amino acid side chain has an amino group? K

Which amino acids have basic functional groups? RHK

### $\mathbf{pI}$

### Question 5: Calculating pI of a peptide

A tripeptide formed from tyrosine, valine, and glycine, in the order as stated. Use the following pKa values:  $\alpha$ -COOH = 2.2,  $\alpha$ -NH<sub>3</sub><sup>+</sup> = 9.4, tyrosine side chain OH = 10.5.

(a) Draw the tripeptide and clearly label where the N-terminus and C-terminus are at pH 7.

$$(N-term) NH_3^+ - Tyr - Val - Gly - COOH (C-term)$$

(b) Calculate the charge of this tripeptide at pH 7.

Compare pKa and pH of each ionizable group:

N-term pKa  $9.4 > \text{pH 7} \rightarrow \text{protonated}$ , charge = +1

C-term pKa  $2.2 < \text{pH } 7 \rightarrow \text{deprotonated}, \text{ charge} = -1$ 

Tyrosine side chain pKa  $10.5 > \text{pH 7} \rightarrow \text{protonated}$ , charge = 0 (protonated form, -OH, carries neutral charge)

Overall charge: 0

(c) Calculate the pI of this tripeptide at pH 7.

Order all the pKa values:

C-term 2.2

N-term 9.4

Tyr 10.5

Always assume full protonation at the beginning (pH < pKa). When the molecule is fully protonated, the overall charge is +1 (neutral C-terminus and tyrosine, positive N-terminus). As the pH increases, the C-term deprotonates first (pKa 2.2), then the N-term (pKa 9.4), and finally the side chain of tyrosine (pKa 10.5). The pI is the average of the two pKa values that surround the zero charge state.

+1

C-term 2.2

0

N-term 9.4

-1

Tyr 10.5

-2

The flanking pKas at charge 0 are 2.2 and 9.4.

$$\frac{2.2 + 9.4}{2} = 5.8$$

The pKa at pH 7 of the peptide is 5.8.

(d) Will you be able to use UV light absorbance at 280 nm to detect your tripeptide? Why or why not?

Yes, because the tripeptide contains a tyrosine side chain, which has a phenolic ring that absorbs UV light at 280 nm. The other two amino acids (valine and glycine) do not absorb UV light at this wavelength.