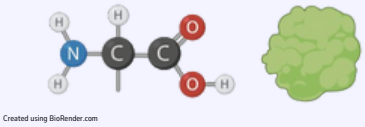
#2: Amino Acids

BIOCHEM2280

What are Amino Acids?

- **Amino acids** (more properly known as alpha-amino acids) are the building blocks of proteins
- In the human body there are 20 amino acids which form the proteins we require to carry out basic cellular functions
- Knowing amino acid structure is vital in understanding protein behavior and interactions



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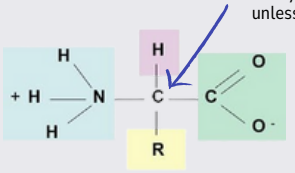
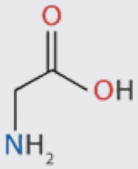
Basic Structure

- The 4 basic constituents of an amino acid are:
  1. **Alpha amino group**
  2. **Alpha carboxyl**
  3. **Hydrogen atom**
  4. **R group (side chain)**

alpha carbon
- always chiral unless in glycine



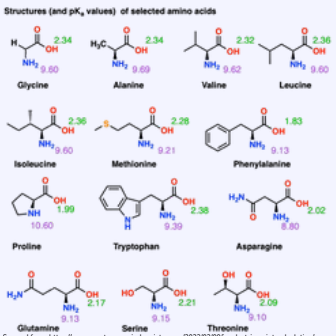
- Since amino acids have 4 different substituents bound to a central carbon, **stereoisomers** exist and are named using *D- and L- nomenclature*
  - All amino acids have a **chiral alpha carbon** except glycine



Glycine

Ionization of Amino Acids

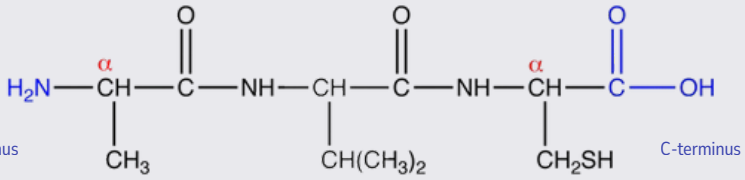
- Depending on the pH which an amino acid is exposed to, weakly acidic or basic groups may ionize which can cause the association/dissociation of protons (H^+ ions)
- **pKa**: a measure describing an acid's tendency to ionize
  - The greater the pKa, the weaker the acid (less likely to completely dissociate)
  - The lower the pKa the stronger the acid (more likely to completely dissociate)



Sourced from: https://www.masterorganicchemistry.com/2023/02/09/isoelectric-point-calculation/

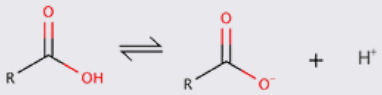
Calculations with pKa

- Since weak acids and bases do not completely dissociate, they exist in equilibrium with their protonated and deprotonated states
- In the structure of amino acids, the **C-terminus (RCOOH group)** is considered a *weak acid* and the **N-terminus (RNH3)** is considered a *weak base*



- The **equilibrium equation for the C-terminus** of an amino acid is:

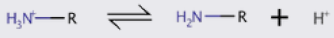
$$Ka = \frac{[H^+][RCOO^-]}{[RCOOH]}$$



  - For the C-terminus, when the pH decreases (Increasing H^+), you will have an increase in the protonated form (RCOOH) and a decrease in the ionized form (RCOO-)

- The **equilibrium equation for the N-terminus** of an amino acid is:

$$Ka = \frac{[H^+][RNH2]}{[RNH3+]}$$



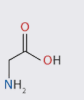
  - For the N-terminus, when pH decreases (Increasing H^+), you will have an increase in the ionized form (RNH3+) and a decrease in the deprotonated form (RNH2)
- As you can see from above, pH will alter the ionization states of functional groups attached to the amino acid
- Amino acids are **amphoteric**, meaning they can act as either acids or bases (Because they have both acidic and basic functional groups)
  - Because of this, they can exist as **Zwitterions** (A molecule carrying both positive and negative charges)

- Since amino acids can hold charges, the **net charge** of an amino acid can be calculated when some information is known
  - *The net charge of an amino acid is the sum of all the charges on an amino acid*

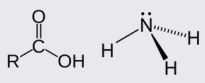
<u>Net charge can be calculated following these steps:</u>

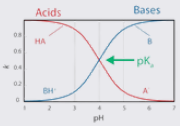
1. Identify ionizable groups
2. Determine pH of solution and pKa values for each ionizable group
   - pKa values of ionizable -R groups (AKA pKR) are typically provided, but it is important to remember the pKa of the carboxyl group (AKA pK1) which is 2.34 and the amino group (AKA pK2) which is 9.6
3. Determine protonation status of ionizable groups
   - When the pH is higher than the pKa, the group will be predominantly deprotonated and thus the group's charge will be equal to its charge in the deprotonated state
   - When the pH is lower than the pKa, the group will be predominantly protonated and thus the group's charge will be equal to its charge in the protonated state
   - When the pH is equal to the pKa, then the group's charge will be the average of the charges in the protonated and deprotonated state
4. Add up charges of ionizable groups

Example:



@ pH 7





Sourced from: https://www.acdlabs.com/blog/improve-chromatographic-separations-consider-mobile-phase-ph-analyte-pka/

+1 (NH3+) + (-1) (COO-) = 0

1. Glycine's ionizable groups are the amino and carboxyl groups
2. The pKa of -COOH is 2.34 and the pKa of -NH3+ is 9.6
3. The pH is higher than the pKa of -COOH so it's deprotonated but it'd lower than -NH3 so it is protonated
4. Therefore the net charge of glycine at pH 7 is 0

- The **Henderson-Hasselbalch equation** can be used to determine the exact ratio of protonated ionizable group to deprotonated ionizable group:

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

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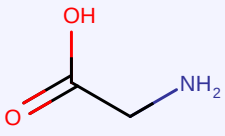
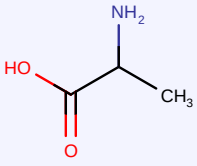
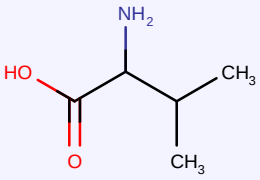
Non-Polar Amino Acids



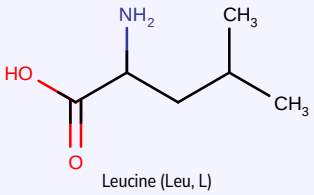
Glycine (Gly, G)



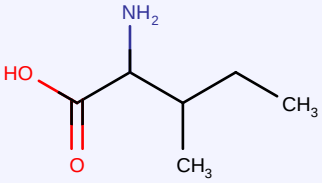
Alanine (Ala, A)



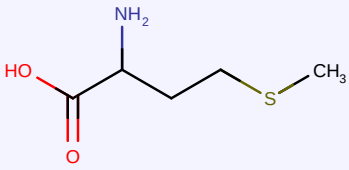
Valine (Val, V)



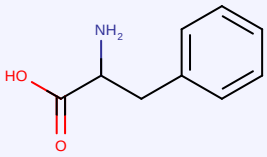
Leucine (Leu, L)



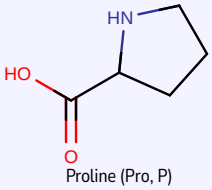
Isoleucine (Ile, I)



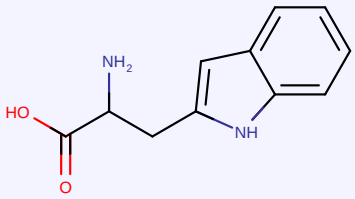
Methionine (Met, M)



Phenylalanine (Phe, F)

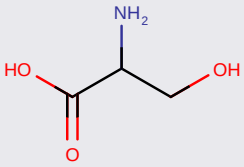


Proline (Pro, P)

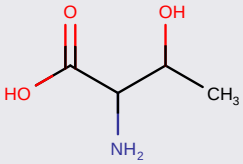


Tryptophan (Trp, W)

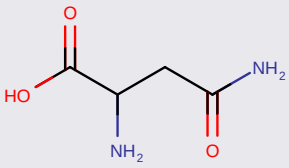
Non-Polar Amino Acids



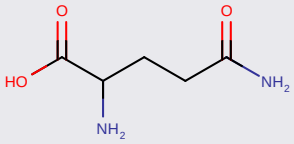
Serine (Ser, S)



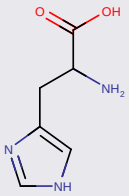
Threonine (Thr, T)



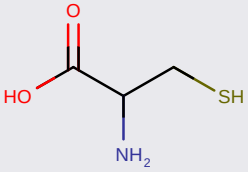
Asparagine (Asn, N)



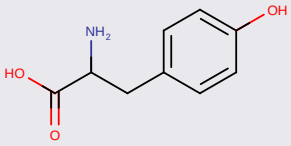
Glutamine (Gln, Q)



Histidine (His, H)

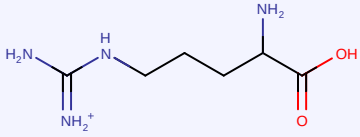


Cysteine (Cys, C)

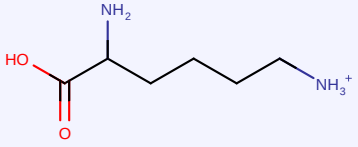


Tyrosine (Tyr, Y)

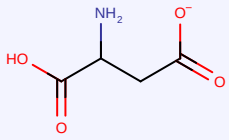
Ionization of Amino Acids



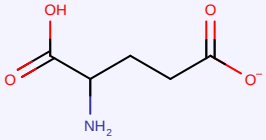
Lysine (Lys, K)



Arginine (Arg, R)



Aspartic Acid (Asp, D)



Glutamic Acid (Glu, E)

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-The WebStraw team

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Note: Marvin was used for drawing, displaying and characterizing chemical structures, substructures and reactions, Marvin 24.4.1, Chemaxon (https://www.chemaxon.com)

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