

# BIO-ORGANIC CHEMISTRY

## (Organic Chemistry for Biology Students)

### (SQBS 1603)

## Basic Compounds in Biomolecules: Amino Acids in Protein

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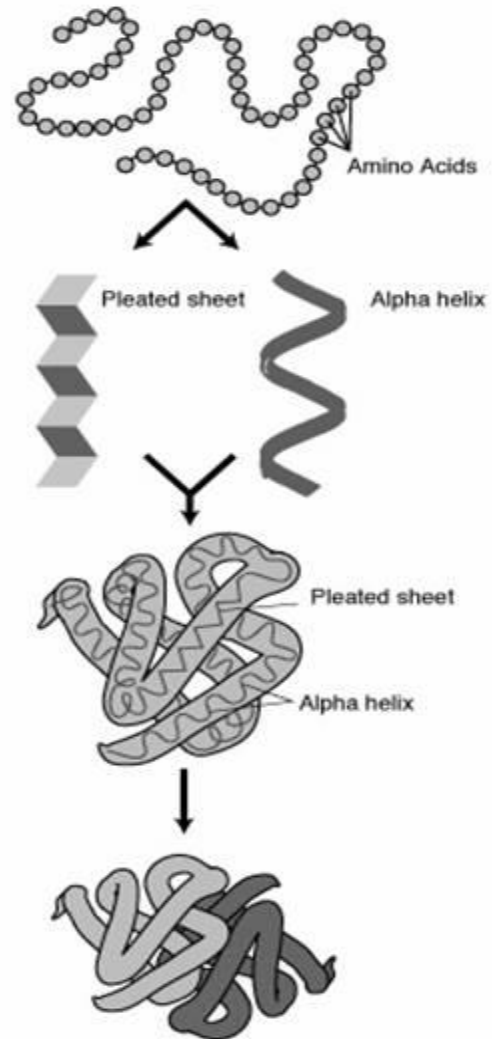
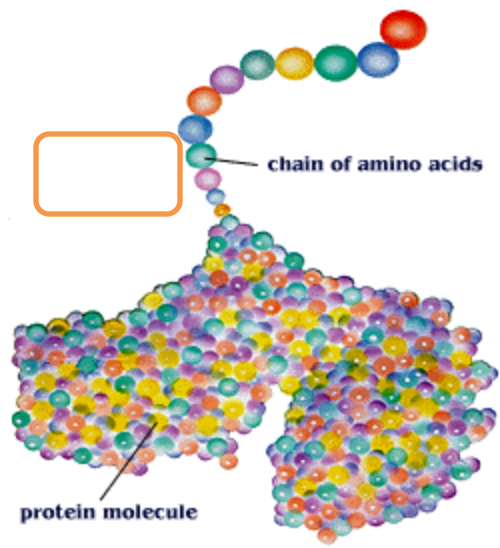
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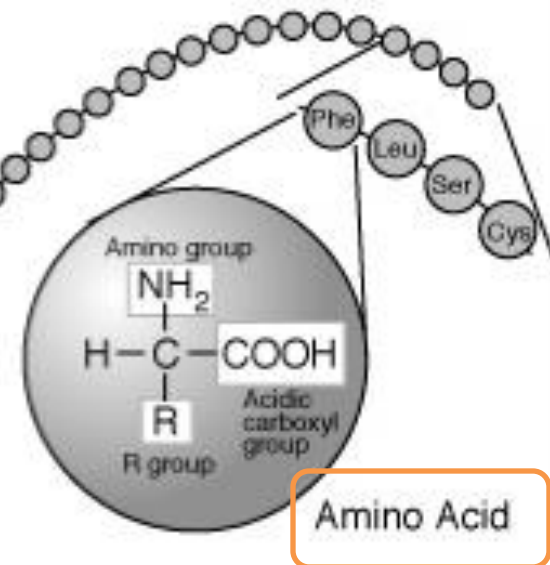
# Protein



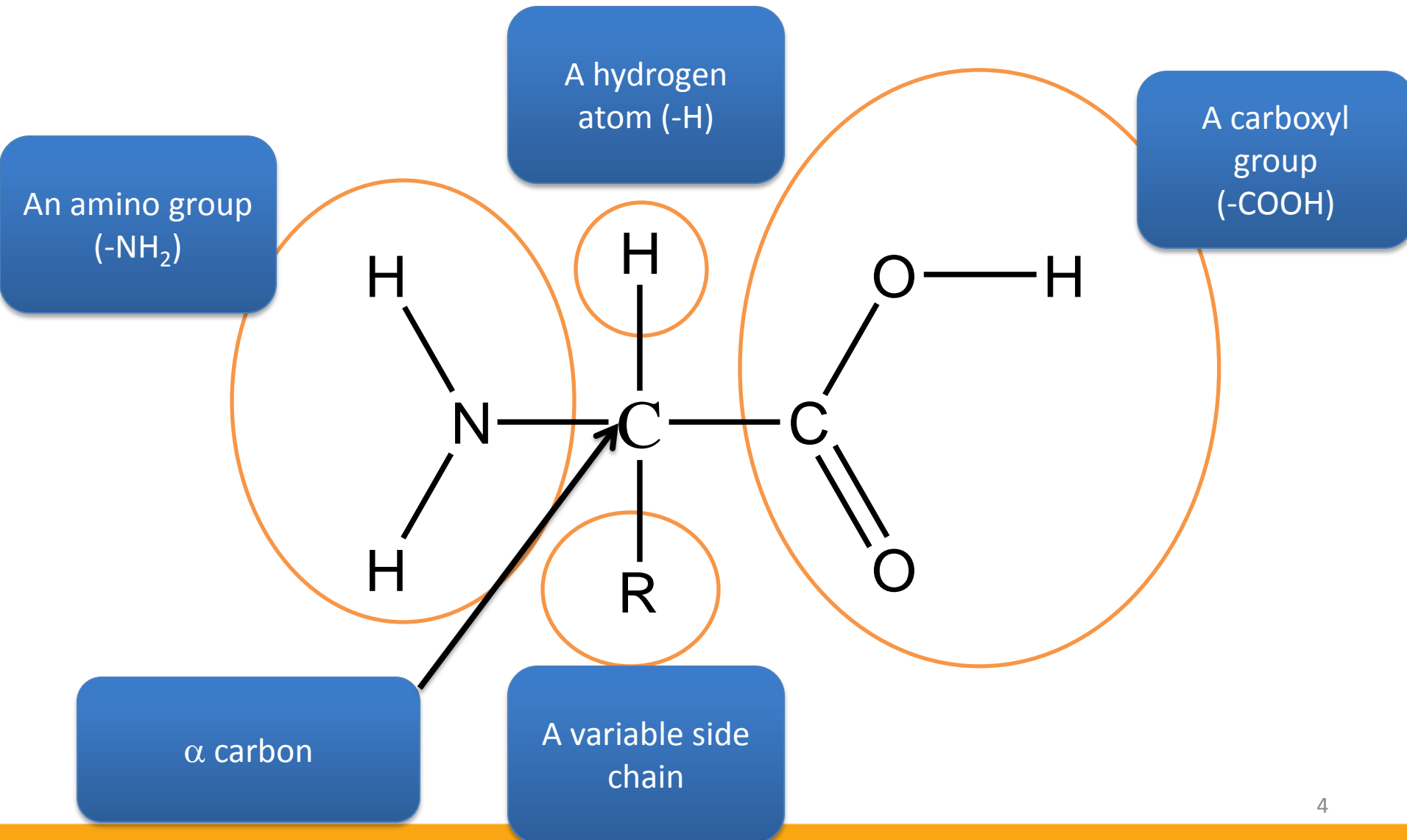
# Protein



Primary protein structure  
is sequence of a chain of amino acids

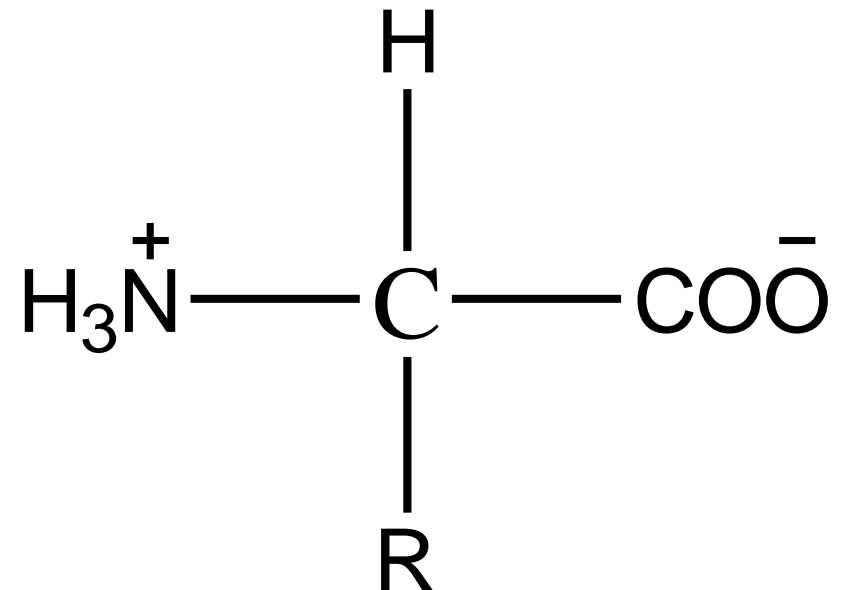
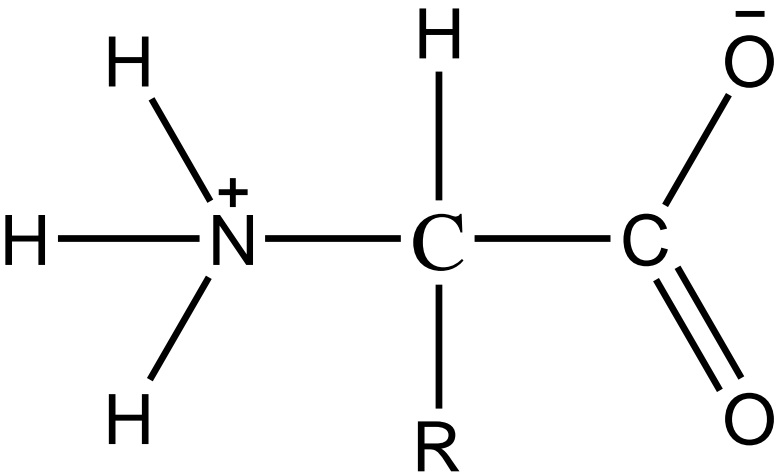


# Amino acid



# Amino acid

Ionized form of amino acid:



# Amino acid

## The 20 common naturally occurring amino acids

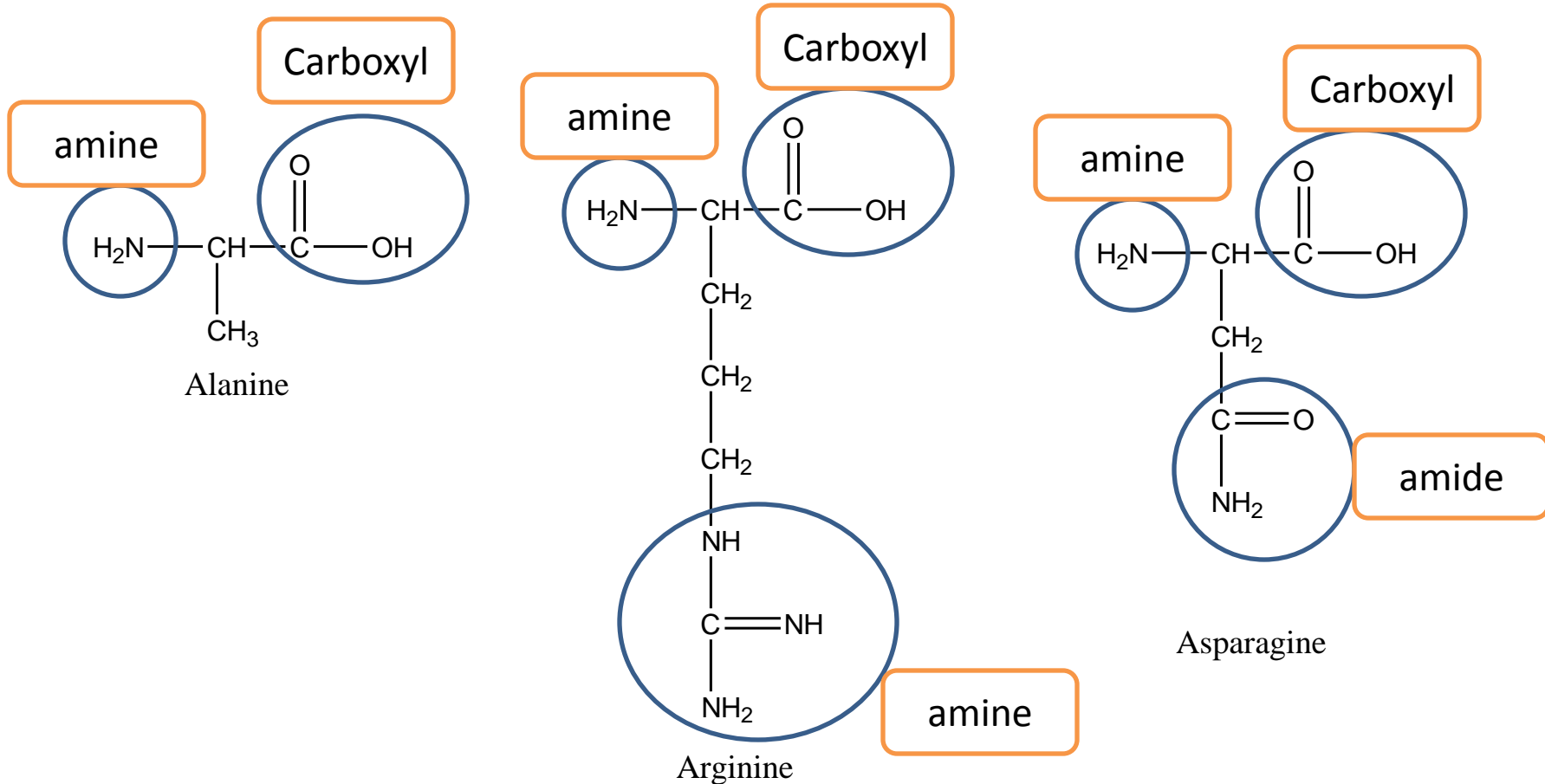
Name	Abbreviations	symbol	Name	Abbreviations	symbol
Glycine	Gly	G	Cysteine	Cys	C
Alanine	Ala	A	*Methionine	Met	M
*Valine	Val	V	Asparagine	Asn	N
*Leucine	Leu	L	Glutamine	Gln	Q
*Isoleucine	Ile	I	*Tryptophan	Trp	W
*phenylalanine	Phe	F	Aspartic acid	Asp	D
Proline	Pro	P	Glutamic acid	Glu	E
Serine	Ser	S	*Lysine	Lys	K
*Threonine	Thr	T	*Arginine	Arg	R
tyrosine	Tyr	Y	PHistidine	His	H

\*Essential amino acids

# The 20 common naturally occurring amino acids

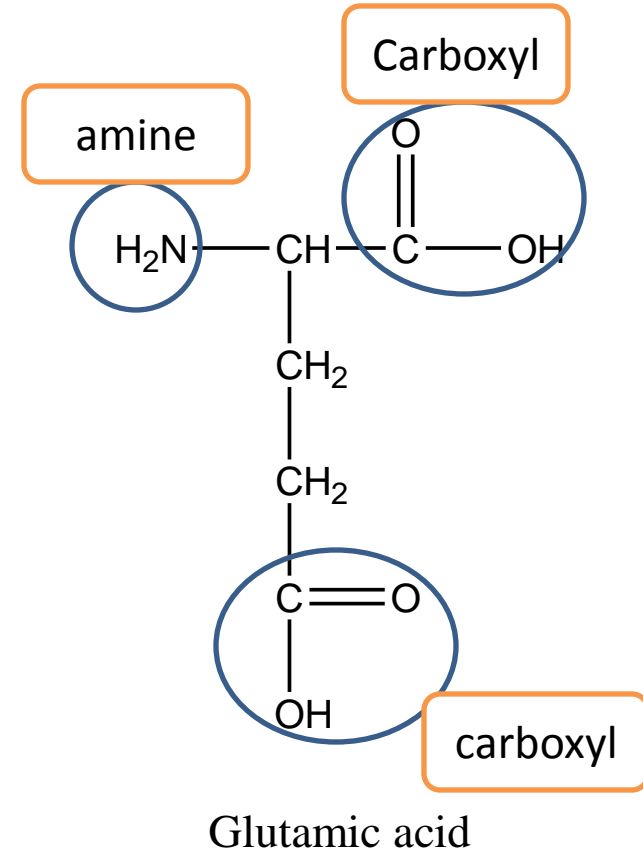
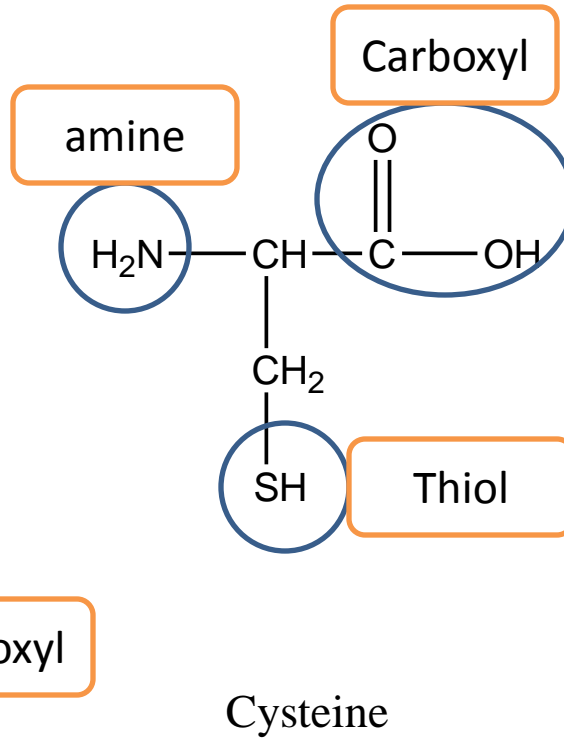
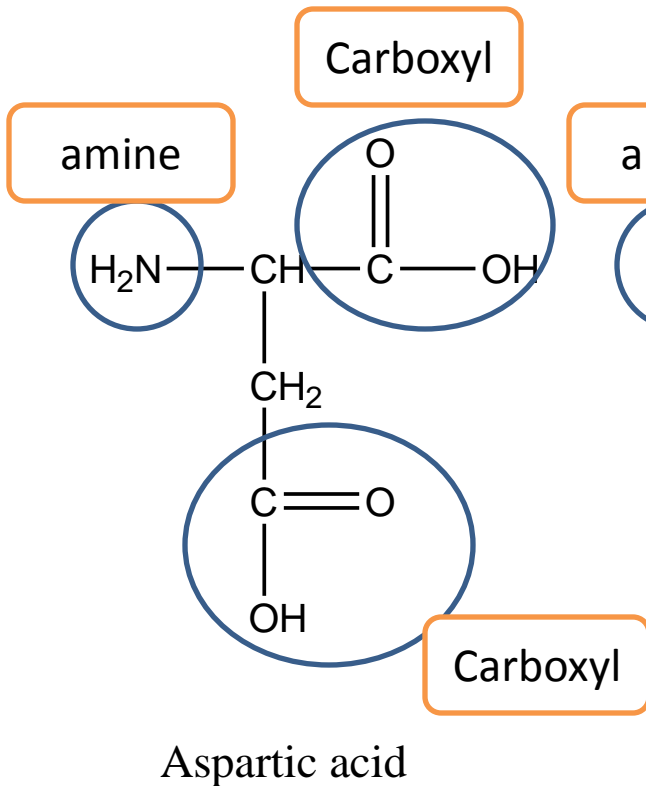
	NONPOLAR, HYDROPHOBIC	R GROUPS	POLAR, UNCHARGED	
Alanine Ala A MW = 89	$\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH}_3 \end{array}$		$\begin{array}{c} \text{H} - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Glycine Gly G MW = 75
Valine Val V MW = 117	$\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH} \begin{array}{l} / \text{CH}_3 \\ \backslash \text{CH}_3 \end{array} \end{array}$		$\begin{array}{c} \text{HO} - \text{CH}_2 - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Serine Ser S MW = 105
Leucine Leu L MW = 131	$\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH}_2 - \text{CH} \begin{array}{l} / \text{CH}_3 \\ \backslash \text{CH}_3 \end{array} \end{array}$		$\begin{array}{c} \text{OH} \\   \\ \text{CH}_3 - \text{CH} - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Threonine Thr T MW = 119
Isoleucine Ile I MW = 131	$\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH} \begin{array}{l} / \text{CH}_3 \\ \backslash \text{CH}_2 - \text{CH}_3 \end{array} \end{array}$		$\begin{array}{c} \text{HS} - \text{CH}_2 - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Cysteine Cys C MW = 121
Phenylalanine Phe F MW = 131	$\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH}_2 - \text{C}_6\text{H}_5 \end{array}$		$\begin{array}{c} \text{HO} - \text{C}_6\text{H}_4 - \text{CH}_2 - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Tyrosine Tyr Y MW = 181
Tryptophan Trp W MW = 204	$\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH}_2 - \text{C}_8\text{H}_6\text{N}_2 \end{array}$		$\begin{array}{c} \text{NH}_2 \\   \\ \text{O} = \text{C} - \text{CH}_2 - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Asparagine Asn N MW = 132
Methionine Met M MW = 149	$\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{S} - \text{CH}_3 \end{array}$		$\begin{array}{c} \text{NH}_2 \\   \\ \text{O} = \text{C} - \text{CH}_2 - \text{CH}_2 - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Glutamine Gln Q MW = 146
Proline Pro P MW = 115	$\begin{array}{c} \text{OOC}^- \\   \\ \text{CH} - \text{CH}_2 - \text{CH}_2 \\   \quad \quad \quad   \\ \text{HN} - \text{CH}_2 \end{array}$		<b>POLAR BASIC</b> $\begin{array}{c} \text{NH}_3^+ - \text{CH}_2 - (\text{CH}_2)_3 - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Lysine Lys K MW = 146
Aspartic acid Asp D MW = 133	<b>POLAR ACIDIC</b> $\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH}_2 - \text{C}(=\text{O})\text{O}^- \end{array}$		$\begin{array}{c} \text{NH}_2 \\   \\ \text{N H}_2^+ = \text{C} - \text{NH} - (\text{CH}_2)_3 - \text{CH} - \text{COO}^- \\   \\ \text{N H}_3^+ \end{array}$	Arginine Arg R MW = 174
Glutamine acid Glu E MW = 147	$\begin{array}{c} \text{OOC}^- \\   \\ \text{H}_3\text{N}^+ - \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{C}(=\text{O})\text{O}^- \end{array}$		$\begin{array}{c} \text{C} = \text{CH}_2 - \text{CH} - \text{COO}^- \\ / \quad \quad \quad   \\ \text{HN} \quad \quad \quad \text{N H}_3^+ \end{array}$	Histidine His H MW = 155

# Functional group in Amino Acid

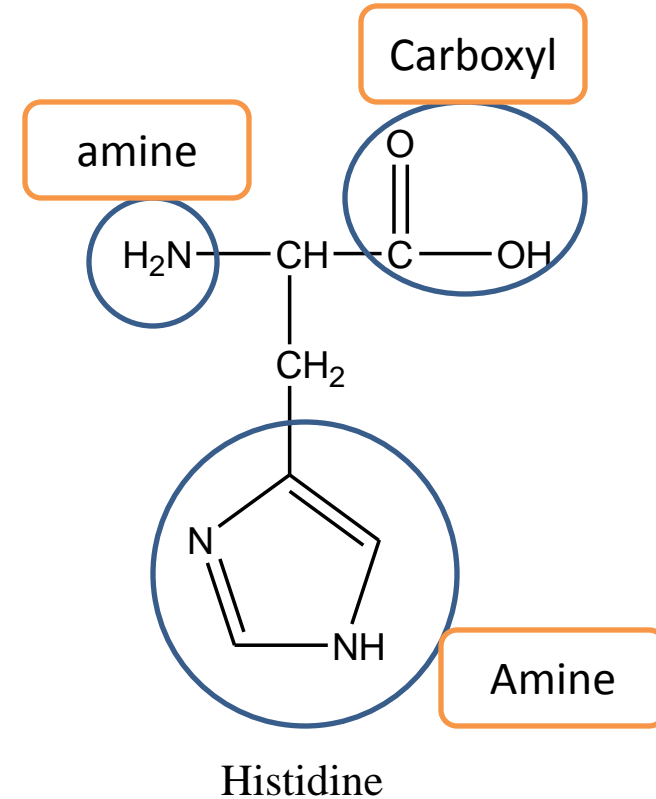
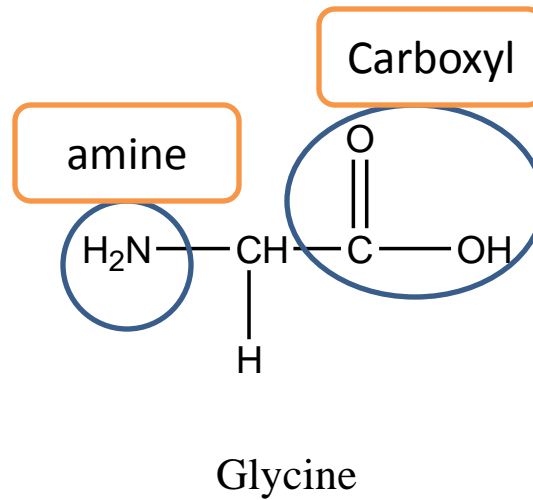
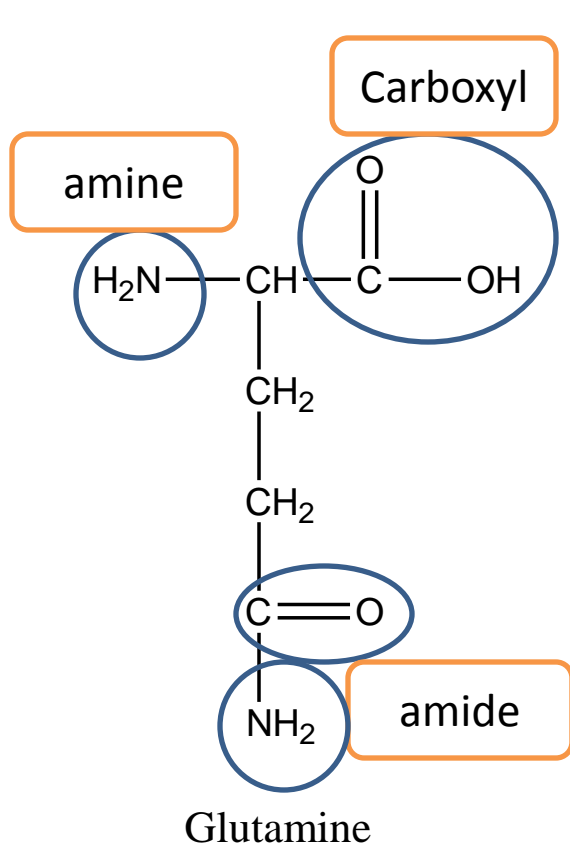




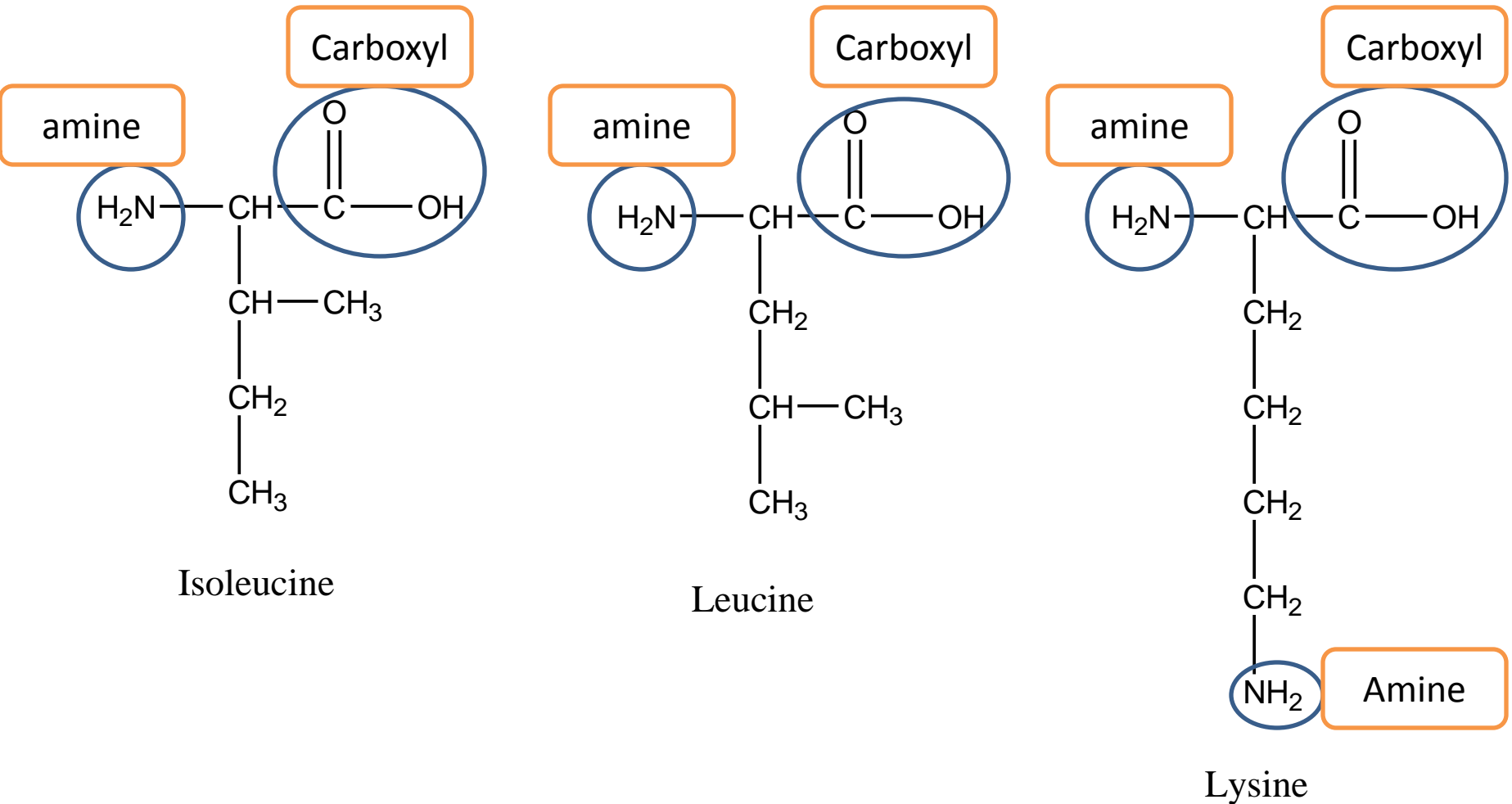
# Functional group in Amino Acid



# Functional group in Amino Acid



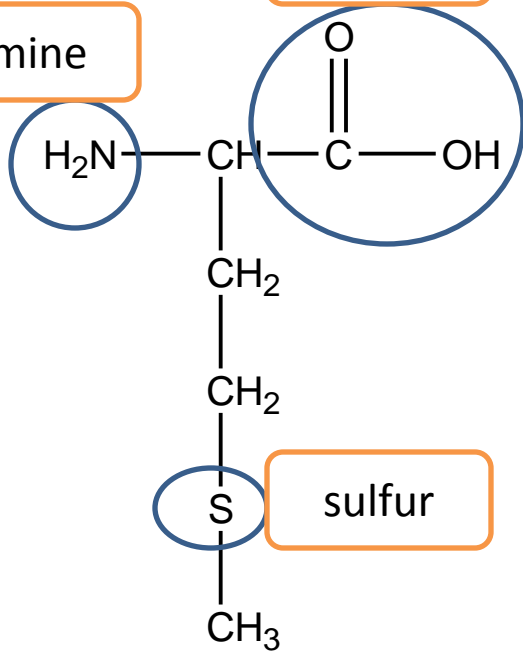
# Functional group in Amino Acid



# Functional group in Amino Acid

amine

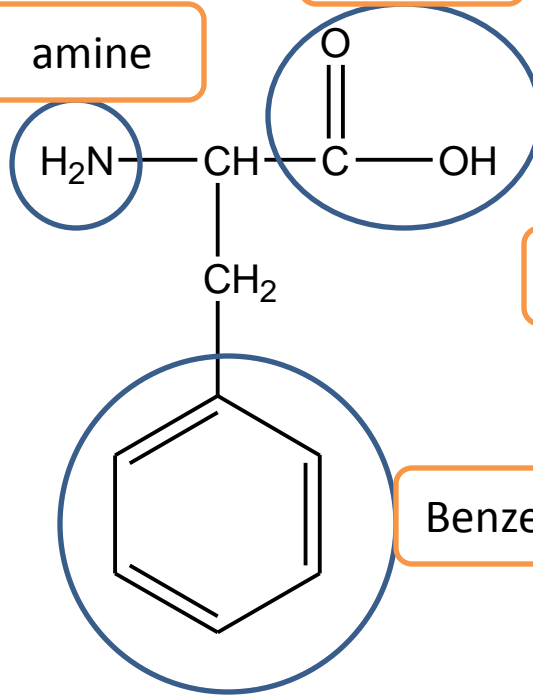
Carboxyl



Methionine

amine

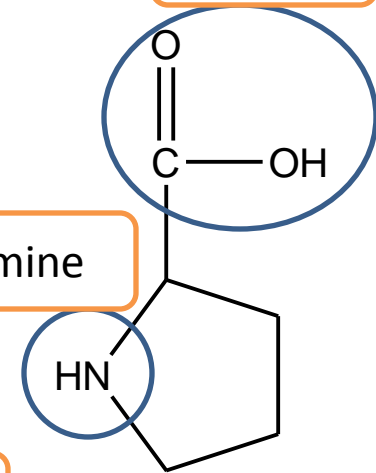
Carboxyl



Phenylalanine

amine

Carboxyl

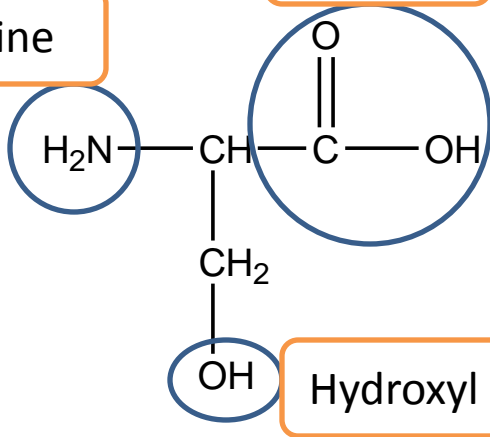


Proline

# Functional group in Amino Acid

amine

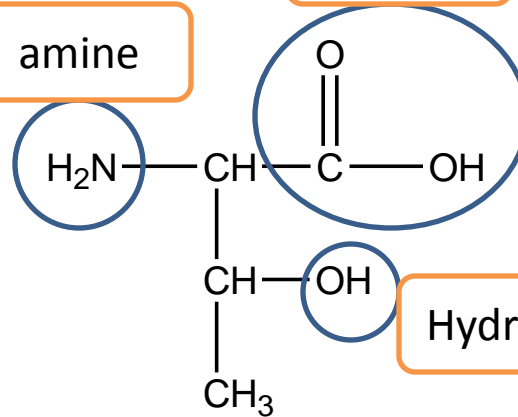
Carboxyl



Serine

amine

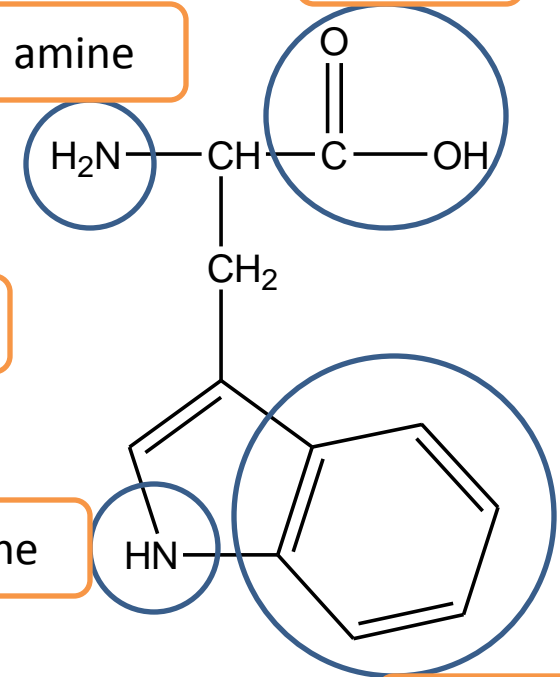
Carboxyl



Threonine

amine

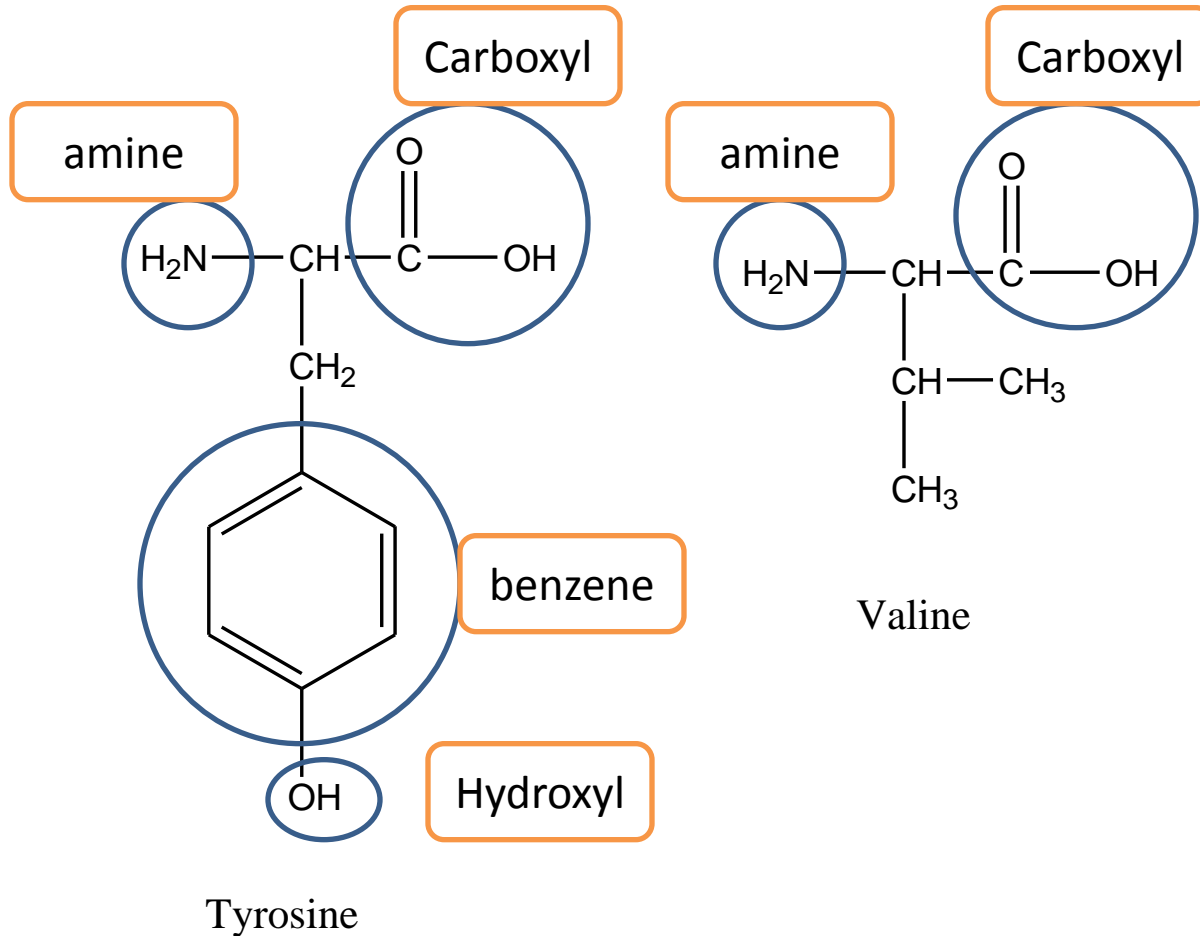
Carboxyl



Tryptophan

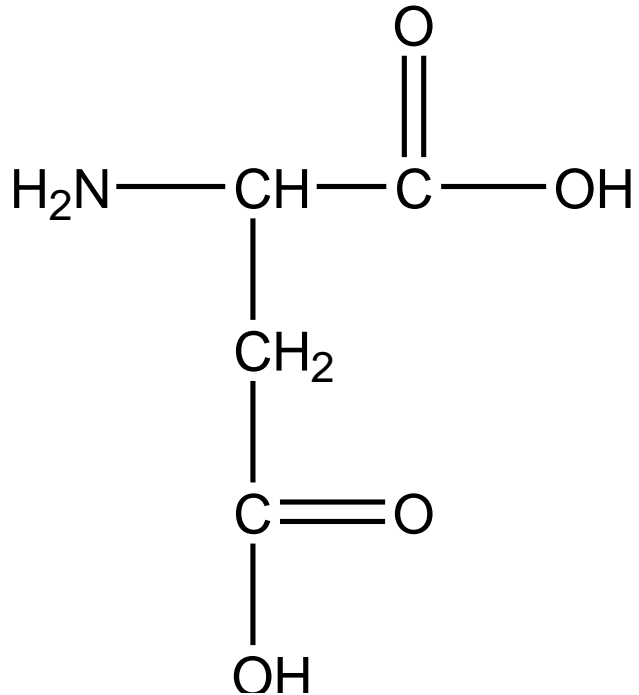
benzene

# Functional group in Amino Acid

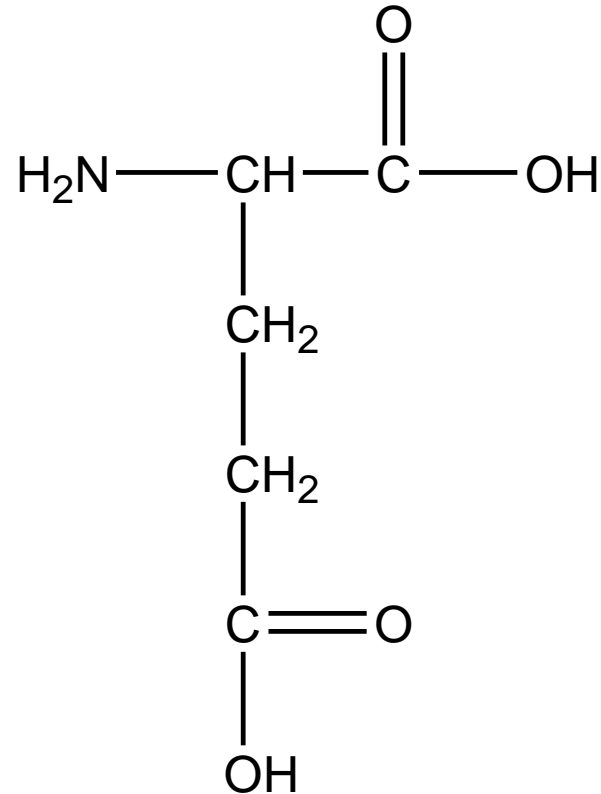


# Amino acid

- **Acidic** amino acids



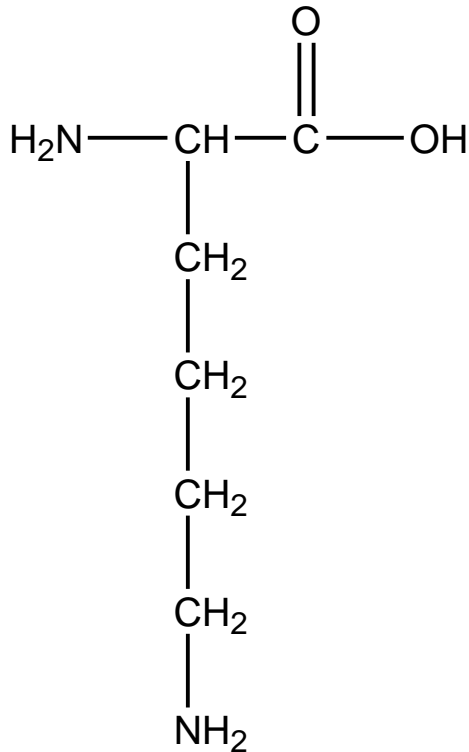
**Aspartic acid**



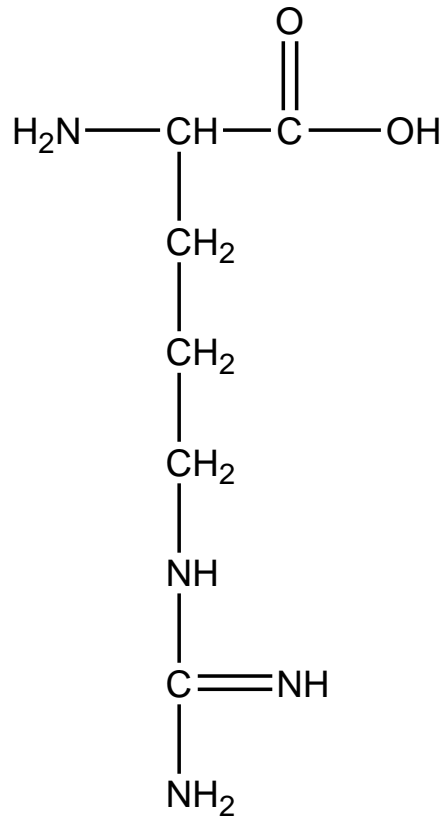
**Glutamic acid**

# Amino acid

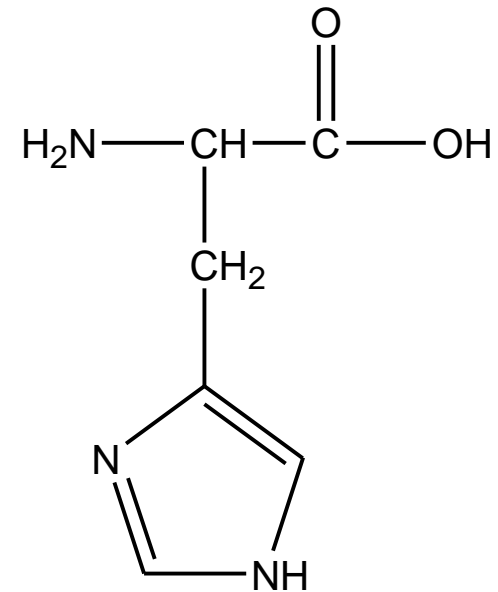
- **Basic** amino acids



Lysine



Arginine



Histidine

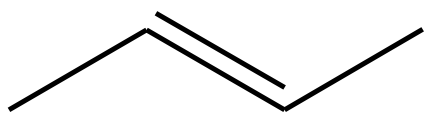


# Isomers

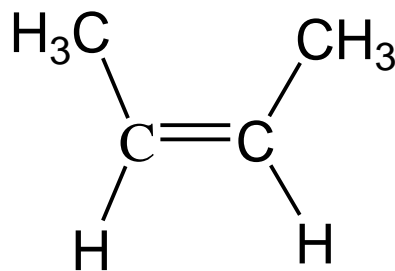
- Groups of compounds that comprise exactly **the same atoms (same chemical composition)** but which have **different structure**, and often different physical and chemical properties too.
- Two types
  1. **Structural Isomers**
  2. **Stereoisomers**

# Stereoisomers

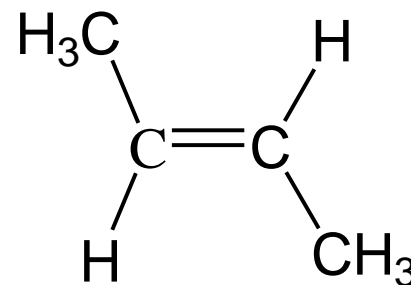
- Stereoisomers possess the same atoms, which exhibit the same connectivity but the composite atoms are oriented differently in space.
  - Different configuration.
  - Differ only in the 3-dimensional arrangement of atoms.
- Two classes
  1. Geometric (cis-trans) isomers.
  2. Enantiomers.



But-2-ene



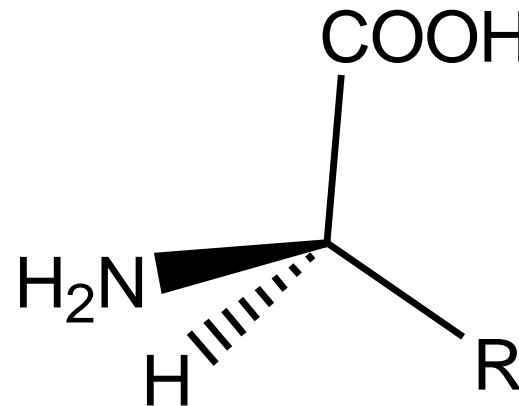
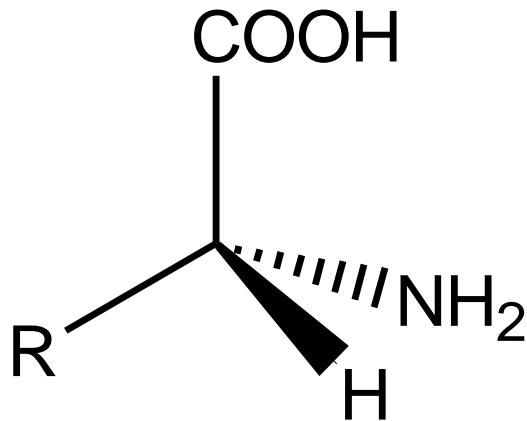
But-2-ene



But-2-ene

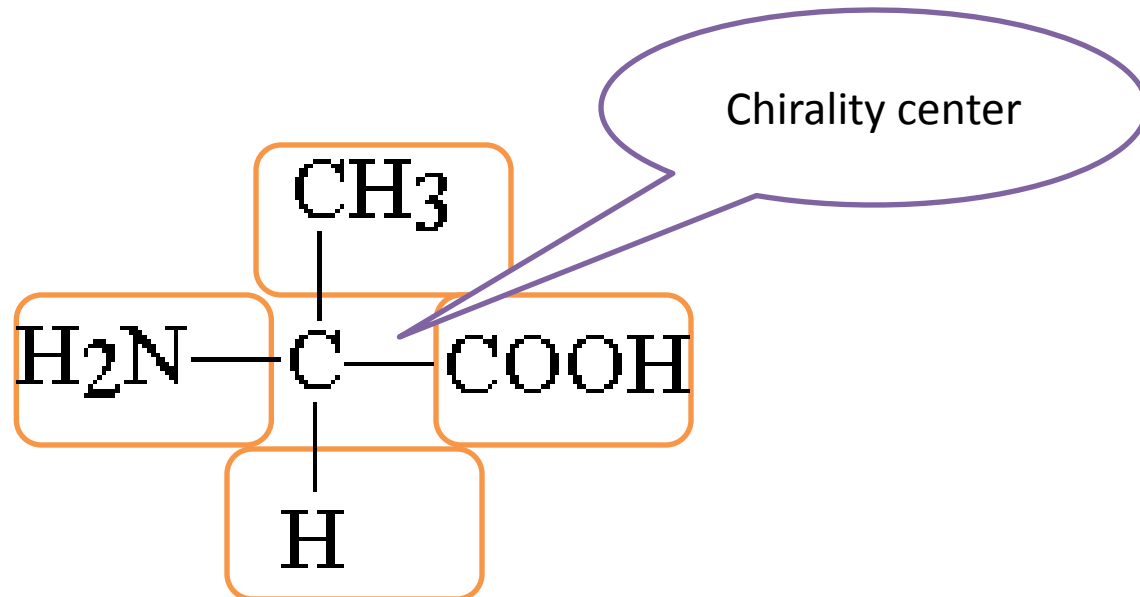
# Enantiomers

- Enantiomers
  - Mirror images that are not superimposable



# Enantiomers

- Chirality center
  - A carbon surrounded by four (4) different groups

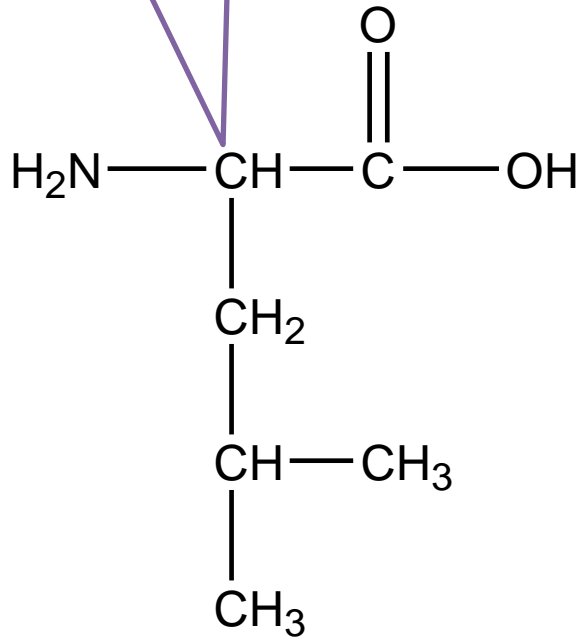


alanine

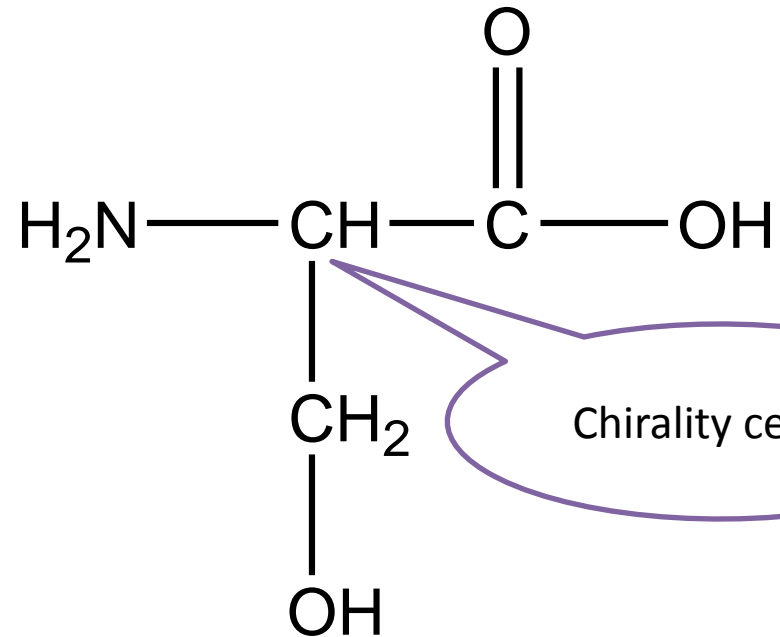
# Enantiomers

- Locate the chirality center for:

Chirality center



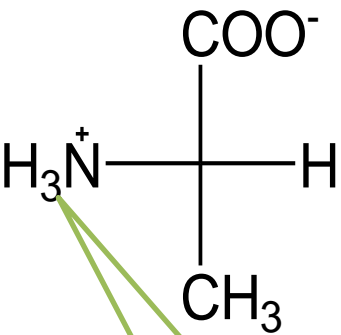
Leucine



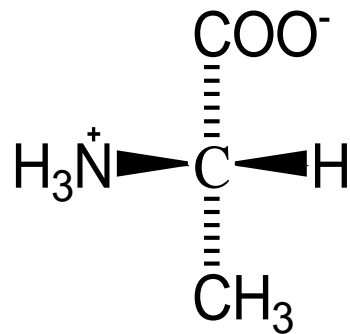
Serine

# Enantiomers

## Fischer projection

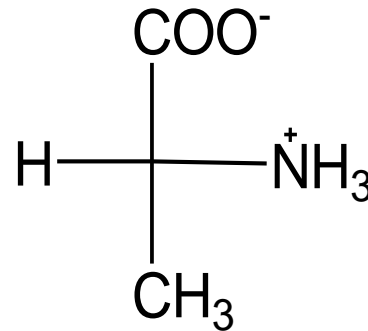


L isomer

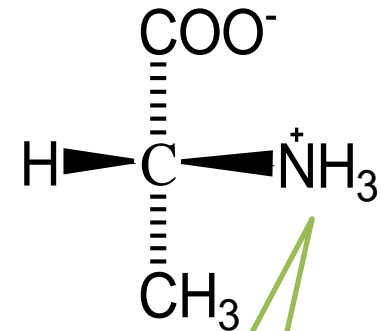


L-alanine

Common naturally  
occurring amino acids



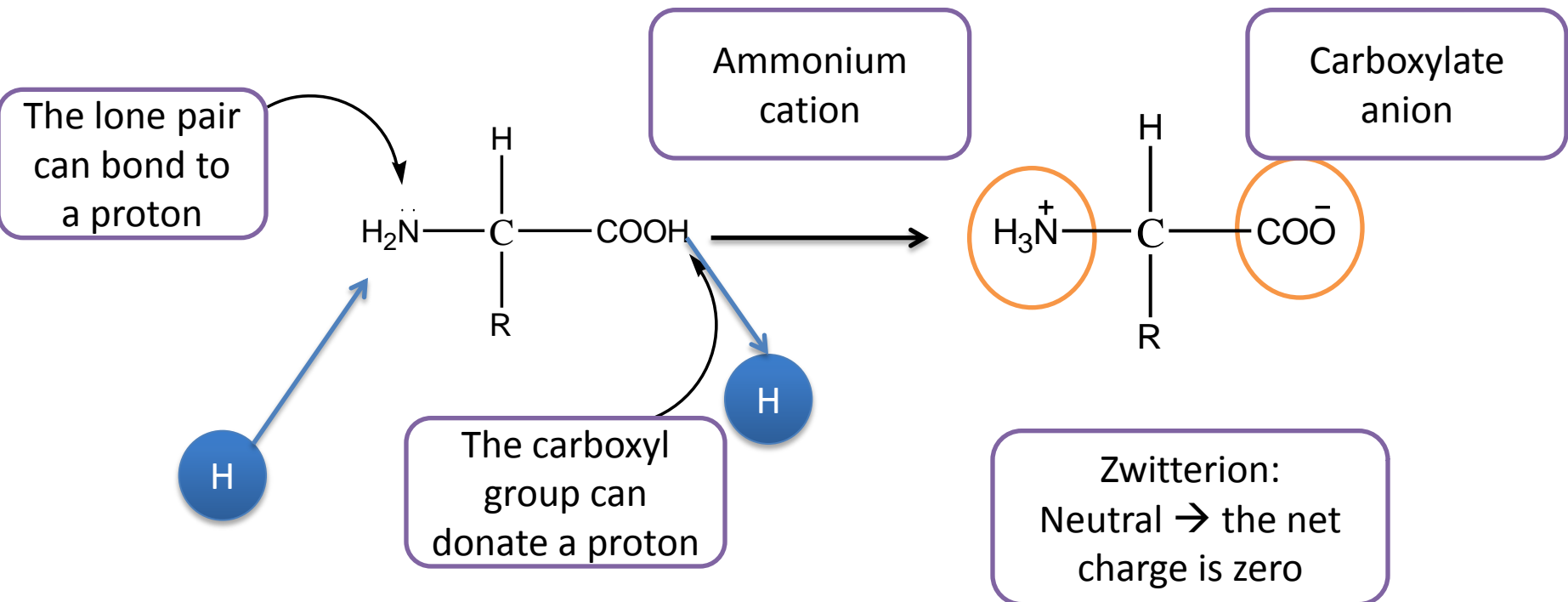
D-alanine



D isomer

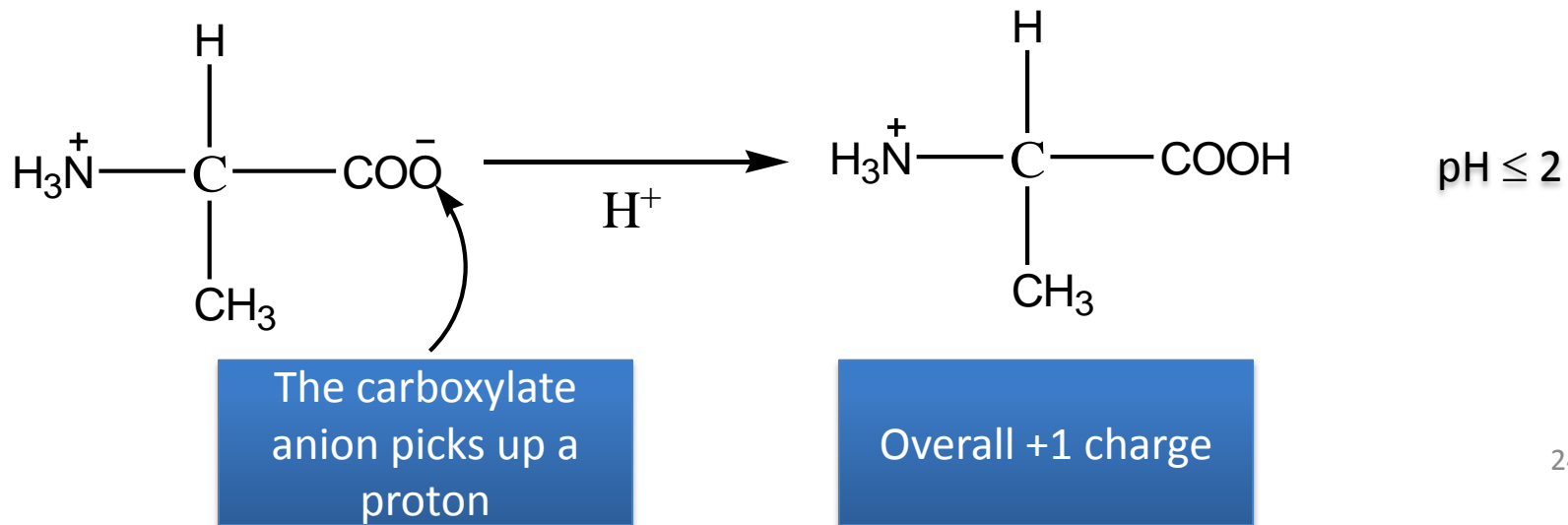
# Acid-base behavior of amino acid

- Basic amino group ( $\text{NH}_2$ )
- Acidic Carboxyl group ( $\text{COOH}$ )



# Acid-base behavior of amino acid

- An amino acid can exist in different forms: depending on the pH of the aqueous solution in which it is dissolved.
- When **strong acid** (pH 2 or less) is added
  - The carboxylate anion gains a proton
  - The amino acid has a net positive charge

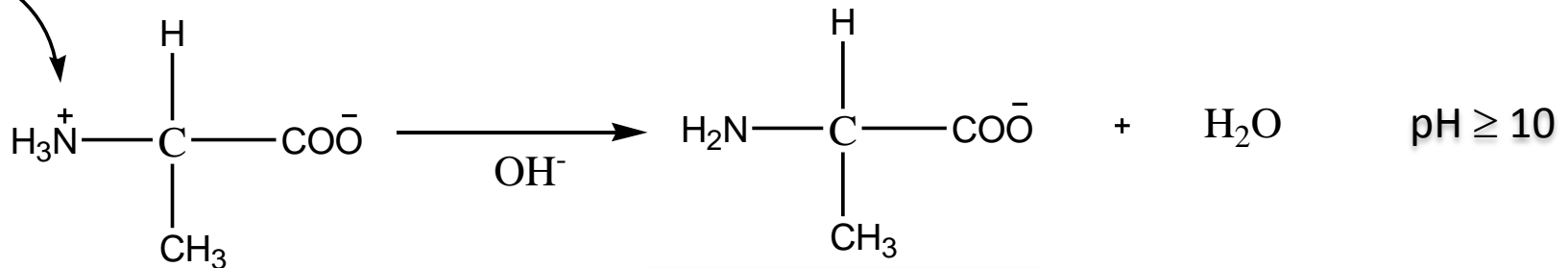




## Acid-base behavior of amino acid

- When strong base (pH 10 to higher) is added
  - The ammonium cation loses a proton
  - The amino acid has a net negative charge

The ammonium cation loses a proton



Overall -1 charge

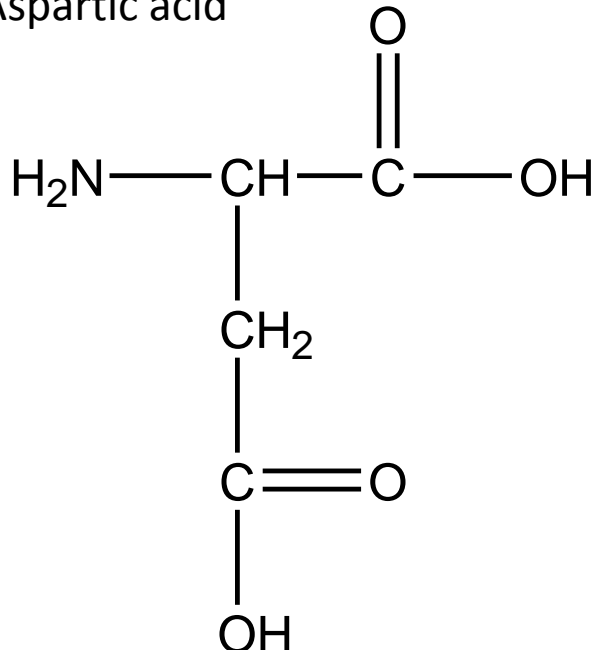
## Acid-base behavior of amino acid

- The pH at which the amino acid exists primarily in its neutral form → *isoelectric point* (*pI*)
- The *pI* of neutral amino acids are generally around 6.
- Acidic amino acids (Asp and Glu)
  - Additional carboxylic group → Can lose additional proton.
  - Have lower *pI* values (around 3)
- Basic amino acids (Arg, His and Lys)
  - Additional basic N → can accept additional proton.
  - Have higher *pI* values (7.6 to 10.8)

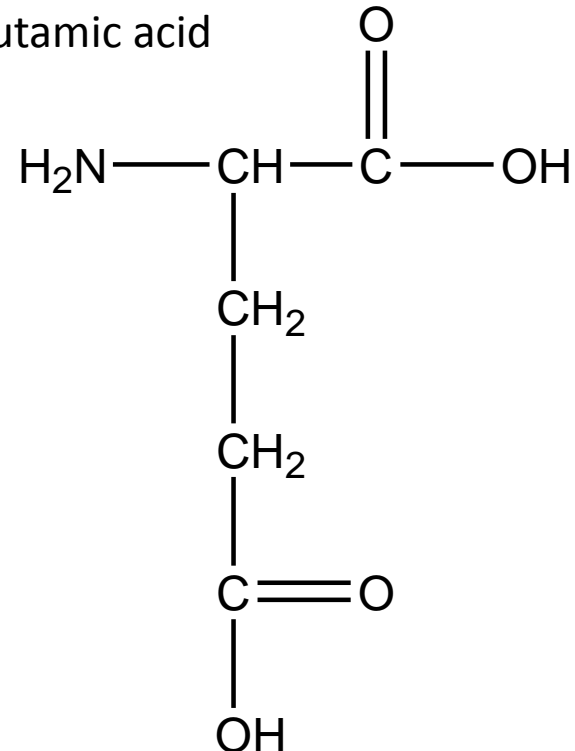
# Acid-base behavior of amino acid

- Acidic amino acids (Asp and Glu)
  - Additional carboxylic group → Can lose additional proton.
  - Have lower pI values (around 3)

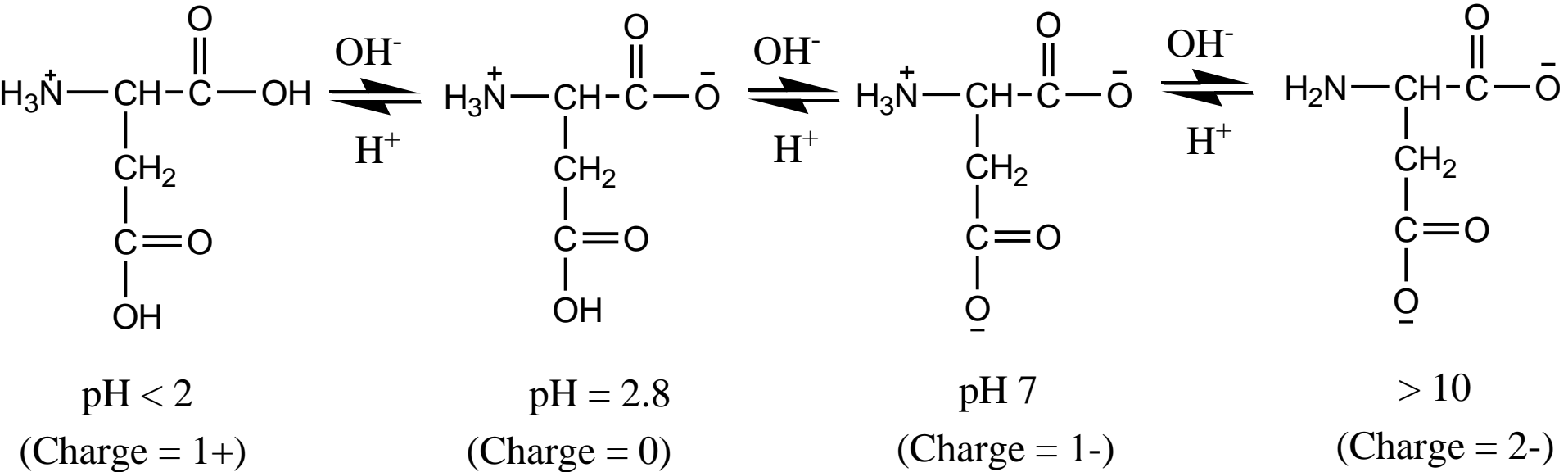
Aspartic acid



Glutamic acid



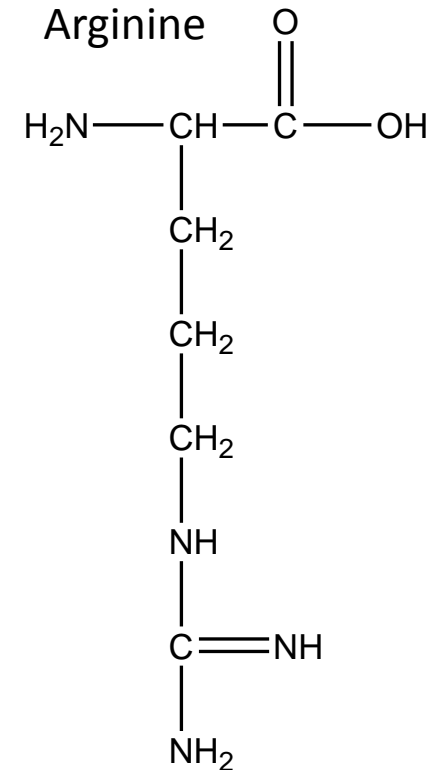
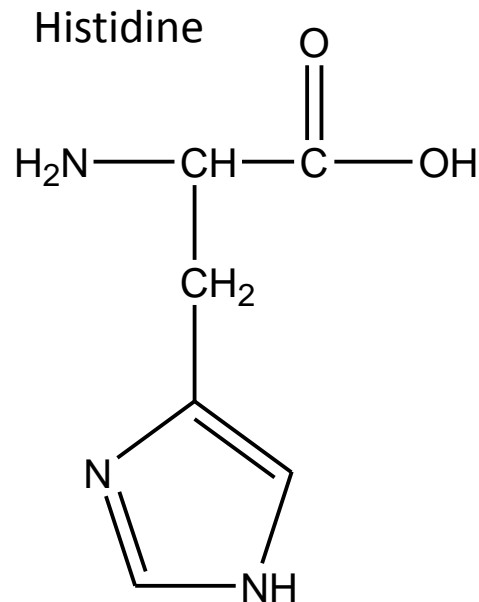
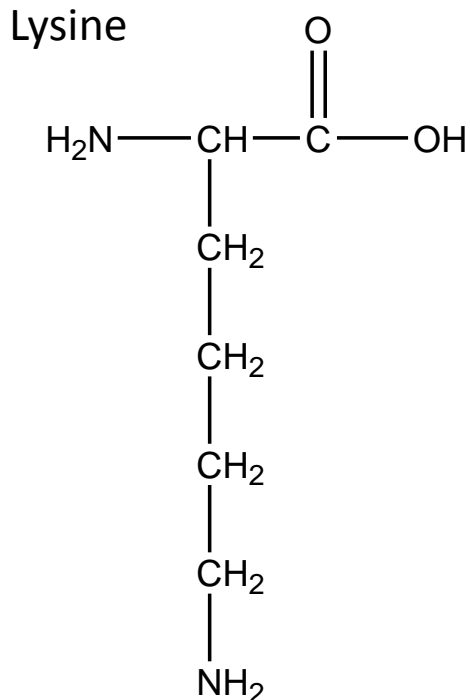
# Acid-base behavior of amino acid




pl of aspartic acid

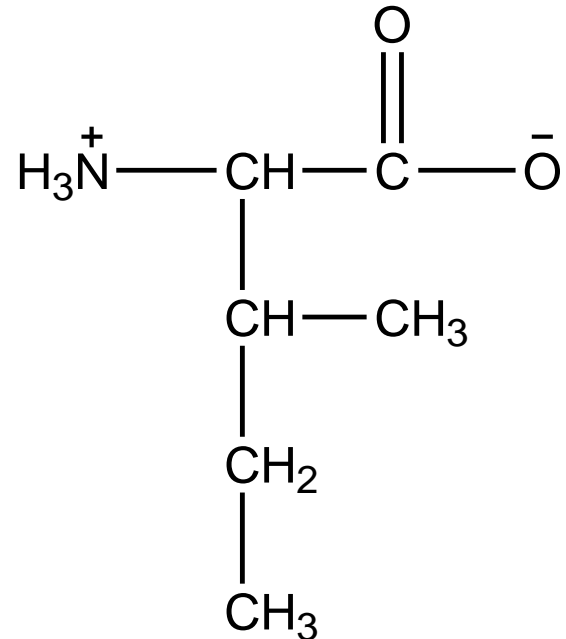
# Acid-base behavior of amino acid

- Basic amino acids (Arg, His and Lys)
  - Additional basic N  $\rightarrow$  can accept additional proton.
  - Have higher pI values (7.6 to 10.8)



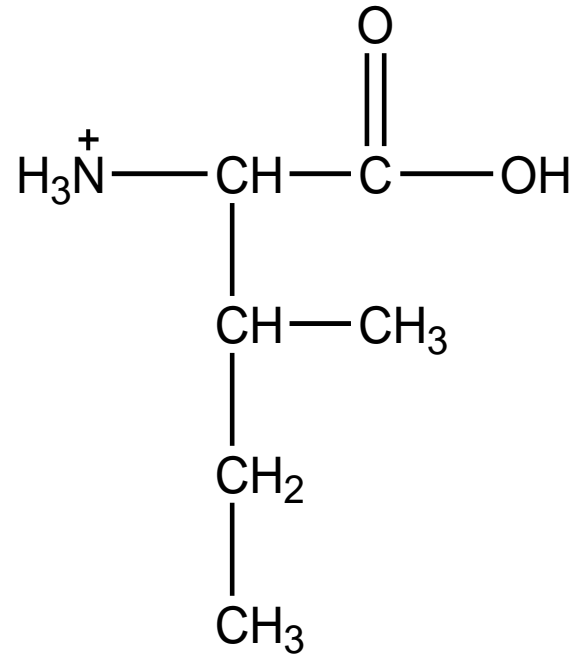
## Acid-base behavior of amino acid

- Structure of the amino acid isoleucine at each pH:
  - pH 6



## Acid-base behavior of amino acid

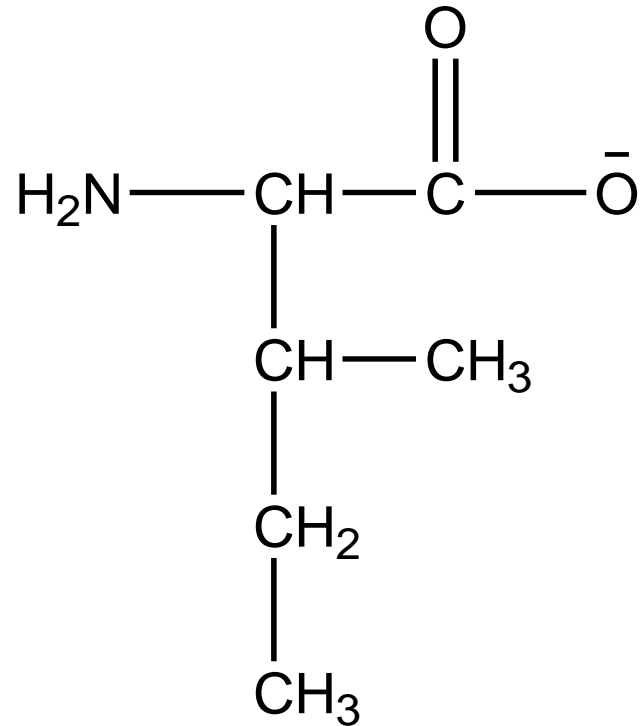
- Structure of the amino acid isoleucine at each pH:
  - pH 2



## Acid-base behavior of amino acid

- Structure of the amino acid isoleucine at each pH:

– pH 11





# REFERENCES

- Crowe, J., Bradshaw, T. and Monk, P. (2006), *Chemistry for the Biosciences: The Essential Concepts*, Oxford University Press, Oxford.
- Horton, H.R., Moran, L.A., Scrimgeour, K.G., Perry, M.D. and Rawn J.D. (2006). *Principles of Biochemistry*, 4<sup>th</sup> Edition. Pearson International Edition.
- Smith, J.G. (2010). *General, Organic and Biological Chemistry*. McGraw-Hill Higher Education.
- Denniston, K.J., Topping, J.J. and Caret, R.L. (2008). *General, Organic and Biochemistry*, 6<sup>th</sup> edition. McGraw-Hill Higher Education.

# MY PROFILE



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Website: <http://www.staff.blog.utm.my/niknizam/>