Donald Voet • Judith G. Voet • Charlotte W. Pratt

Fundamentals of Biochemistry

Second Edition

Chapter 4:

Amino Acids

Chapter 4 Opener Fundamentals of Biochemistry, 2/e

α-amino acids

α-carbon
Carboxylic acid group
Amino group
R group

General structure

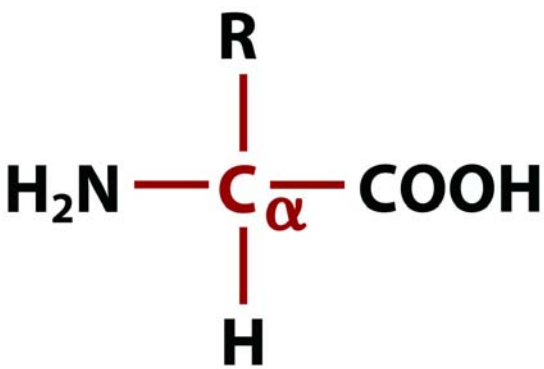

Figure 4-1 Fundamentals of Biochemistry, 2/e
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Zwitterionic (dipolar) form
(at physiological pH)

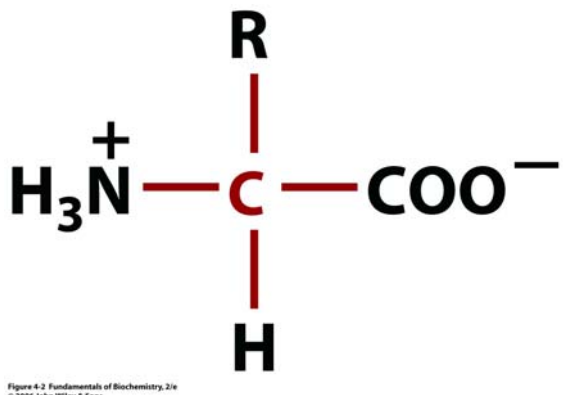

Figure 4-2 Fundamentals of Biochemistry, 2/e
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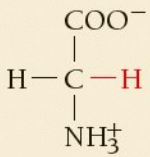
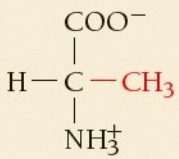
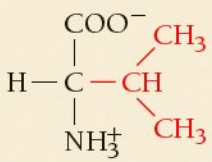
pK_1, pK_2, pK_R

Table 4-1 *Key to Structure.* **Covalent Structures and Abbreviations of the "Standard" Amino Acids of Proteins, Their Occurrence, and the p*K* Values of Their Ionizable Groups**

Name, Three-letter Symbol, and One-letter Symbol	Structural Formula[a]	Residue Mass (D)[b]	Average Occurrence in Proteins (%)[c]	pK_1 α-COOH[d]	pK_2 α-NH_3^+[d]	pK_R Side Chain[d]
Amino acids with nonpolar side chains						
Glycine Gly G		57.0	7.2	2.35	9.78	
Alanine Ala A		71.1	7.8	2.35	9.87	
Valine Val V		99.1	6.6	2.29	9.74	

[a]The ionic forms shown are those predominating at pH 7.0 (except for that of histidine[f]) although residue mass is given for the neutral compound. The C_α atoms, as well as those atoms marked with an asterisk, are chiral centers with configurations as indicated according to Fischer projection formulas (Section 4-2). The standard organic numbering system is provided for heterocycles.

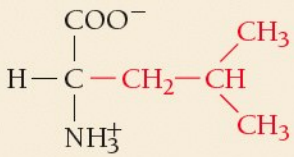
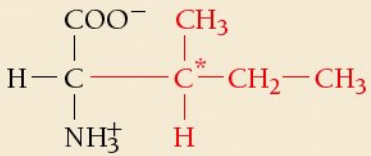
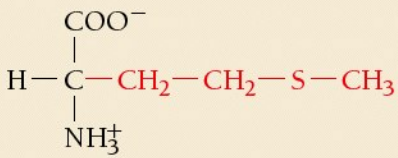
[b]The residue masses are given for the neutral residues. For the molecular masses of the parent amino acids, add 18.0 D, the molecular mass of H_2O, to the residue masses. For side chain masses, subtract 56.0 D, the formula mass of a peptide group, from the residue masses.

[c]Calculated from a database of nonredundant proteins containing 300,688 residues as compiled by Doolittle, R.F. *in* Fasman, G.D. (Ed.), *Predictions of Protein Structure and the Principles of Protein Conformation,* Plenum Press (1989).

[d]Data from Dawson, R.M.C., Elliott, D.C., Elliott, W.H., and Jones, K.M., *Data for Biochemical Research* (3rd ed.), pp. 1–31, Oxford Science Publications (1986).

Table 4-1 part 1 Fundamentals of Biochemistry, 2/e

Table 4-1 *Key to Structure.* **Covalent Structures and Abbreviations of the "Standard" Amino Acids of Proteins, Their Occurrence, and the p*K* Values of Their Ionizable Groups**

Name, Three-letter Symbol, and One-letter Symbol	Structural Formula[a]	Residue Mass (D)[b]	Average Occurrence in Proteins (%)[c]	pK_1 α-COOH[d]	pK_2 α-NH_3^+[d]	pK_R Side Chain[d]
Amino acids with nonpolar side chains						
Leucine Leu L		113.2	9.1	2.33	9.74	
Isoleucine Ile I		113.2	5.3	2.32	9.76	
Methionine Met M		131.2	2.2	2.13	9.28	

[a]The ionic forms shown are those predominating at pH 7.0 (except for that of histidine[f]) although residue mass is given for the neutral compound. The C_α atoms, as well as those atoms marked with an asterisk, are chiral centers with configurations as indicated according to Fischer projection formulas (Section 4-2). The standard organic numbering system is provided for heterocycles.

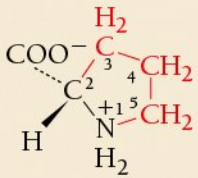
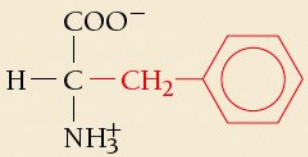
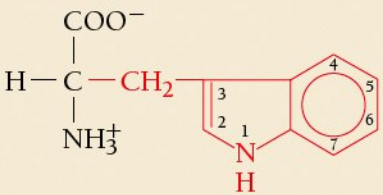
[b]The residue masses are given for the neutral residues. For the molecular masses of the parent amino acids, add 18.0 D, the molecular mass of H_2O, to the residue masses. For side chain masses, subtract 56.0 D, the formula mass of a peptide group, from the residue masses.

[c]Calculated from a database of nonredundant proteins containing 300,688 residues as compiled by Doolittle, R.F. *in* Fasman, G.D. (Ed.), *Predictions of Protein Structure and the Principles of Protein Conformation,* Plenum Press (1989).

[d]Data from Dawson, R.M.C., Elliott, D.C., Elliott, W.H., and Jones, K.M., *Data for Biochemical Research* (3rd ed.), pp. 1–31, Oxford Science Publications (1986).

Table 4-1 part 2 Fundamentals of Biochemistry, 2/e

Table 4-1 *Key to Structure.* **Covalent Structures and Abbreviations of the "Standard" Amino Acids of Proteins, Their Occurrence, and the p*K* Values of Their Ionizable Groups**

Name, Three-letter Symbol, and One-letter Symbol	Structural Formula[a]	Residue Mass (D)[b]	Average Occurrence in Proteins (%)[c]	pK_1 α-COOH[d]	pK_2 α-NH_3^+[d]	pK_R Side Chain[d]
Amino acids with nonpolar side chains						
Proline Pro P		97.1	5.2	1.95	10.64	
Phenylalanine Phe F		147.2	3.9	2.20	9.31	
Tryptophan Trp W		186.2	1.4	2.46	9.41	

[a]The ionic forms shown are those predominating at pH 7.0 (except for that of histidine[f]) although residue mass is given for the neutral compound. The C_α atoms, as well as those atoms marked with an asterisk, are chiral centers with configurations as indicated according to Fischer projection formulas (Section 4-2). The standard organic numbering system is provided for heterocycles.

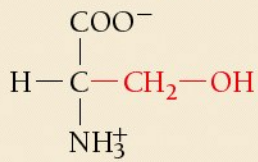
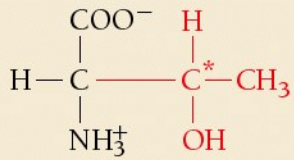
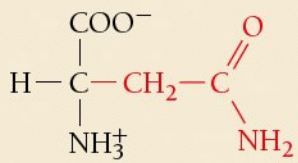
[b]The residue masses are given for the neutral residues. For the molecular masses of the parent amino acids, add 18.0 D, the molecular mass of H_2O, to the residue masses. For side chain masses, subtract 56.0 D, the formula mass of a peptide group, from the residue masses.

[c]Calculated from a database of nonredundant proteins containing 300,688 residues as compiled by Doolittle, R.F. *in* Fasman, G.D. (Ed.), *Predictions of Protein Structure and the Principles of Protein Conformation,* Plenum Press (1989).

[d]Data from Dawson, R.M.C., Elliott, D.C., Elliott, W.H., and Jones, K.M., *Data for Biochemical Research* (3rd ed.), pp. 1–31, Oxford Science Publications (1986).

Table 4-1 part 3 Fundamentals of Biochemistry, 2/e

Table 4-1 (continued)

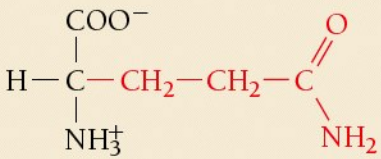
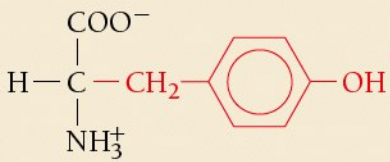
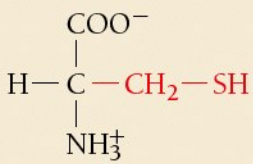
Name, Three-letter Symbol, and One-letter Symbol	Structural Formula[a]	Residue Mass (D)[b]	Average Occurrence in Proteins (%)[c]	pK_1 α-COOH[d]	pK_2 α-NH_3^+[d]	pK_R Side Chain[d]
Amino acids with uncharged polar side chains						
Serine Ser S		87.1	6.8	2.19	9.21	
Threonine Thr T		101.1	5.9	2.09	9.10	
Asparagine[e] Asn N		114.1	4.3	2.14	8.72	

[e]The three- and one-letter symbols for asparagine *or* aspartic acid are Asx and B, whereas for glutamine *or* glutamic acid they are Glx and Z. The one-letter symbol for an undetermined or "nonstandard" amino acid is X.

[f]Both neutral and protonated forms of histidine are present at pH 7.0, since its pK_R is close to 7.0.

Table 4-1 part 4 Fundamentals of Biochemistry, 2/e

Table 4-1 (continued)

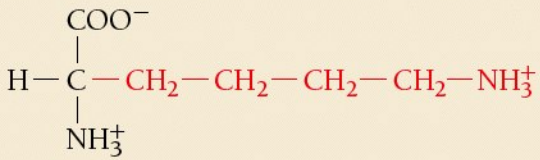
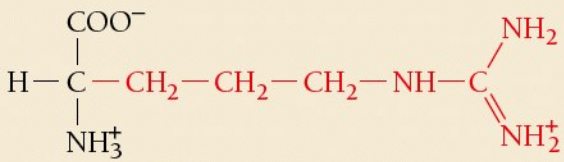
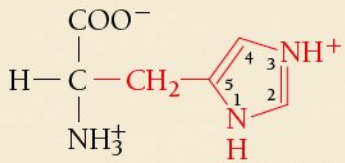
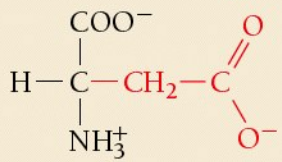
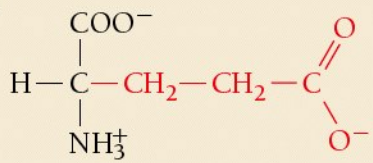
Name, Three-letter Symbol, and One-letter Symbol	Structural Formula[a]	Residue Mass (D)[b]	Average Occurrence in Proteins (%)[c]	pK_1 α-COOH[d]	pK_2 α-NH_3^+[d]	pK_R Side Chain[d]
Amino acids with uncharged polar side chains						
Glutamine[e] Gln Q		128.1	4.3	2.17	9.13	
Tyrosine Tyr Y		163.2	3.2	2.20	9.21	10.46 (phenol)
Cysteine Cys C		103.1	1.9	1.92	10.70	8.37 (sulfhydryl)

[e]The three- and one-letter symbols for asparagine *or* aspartic acid are Asx and B, whereas for glutamine *or* glutamic acid they are Glx and Z. The one-letter symbol for an undetermined or "nonstandard" amino acid is X.

[f]Both neutral and protonated forms of histidine are present at pH 7.0, since its pK_R is close to 7.0.

Table 4-1 part 5 Fundamentals of Biochemistry, 2/e

Table 4-1 (continued)

Name, Three-letter Symbol, and One-letter Symbol	Structural Formula[a]	Residue Mass (D)[b]	Average Occurrence in Proteins (%)[c]	pK_1 α-COOH[d]	pK_2 α-NH_3^+[d]	pK_R Side Chain[d]
Amino acids with charged polar side chains						
Lysine Lys K		128.2	5.9	2.16	9.06	10.54 (ε-NH_3^+)
Arginine Arg R		156.2	5.1	1.82	8.99	12.48 (guanidino)
Histidine[f] His H		137.1	2.3	1.80	9.33	6.04 (imidazole)
Aspartic acid[e] Asp D		115.1	5.3	1.99	9.90	3.90 (β-COOH)
Glutamic acid[e] Glu E		129.1	6.3	2.10	9.47	4.07 (γ-COOH)

[e]The three- and one-letter symbols for asparagine *or* aspartic acid are Asx and B, whereas for glutamine *or* glutamic acid they are Glx and Z. The one-letter symbol for an undetermined or "nonstandard" amino acid is X.

[f]Both neutral and protonated forms of histidine are present at pH 7.0, since its pK_R is close to 7.0.

Table 4-1 part 6 Fundamentals of Biochemistry, 2/e

Amino acids in space filling model

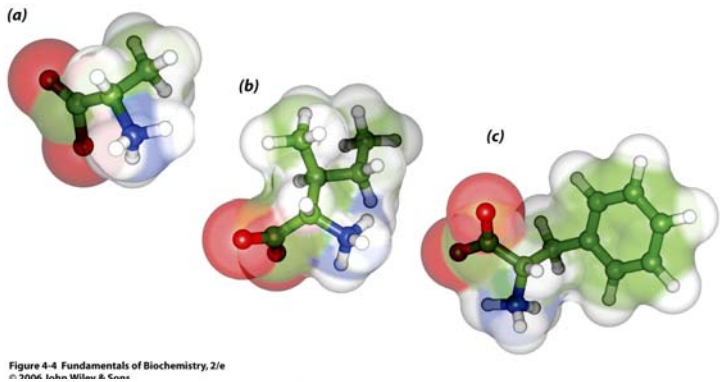


Figure 4-4 Fundamentals of Biochemistry, 2/e
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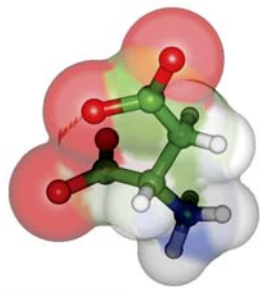

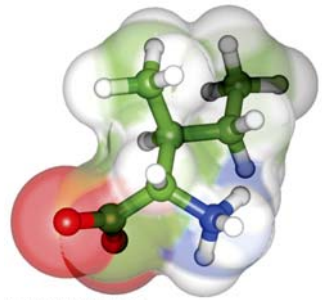

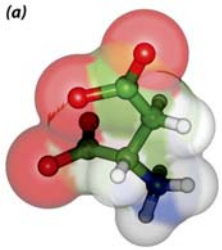

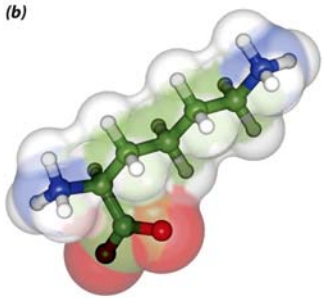

Figure 4-7 Fundamentals of Biochemistry, 2/e
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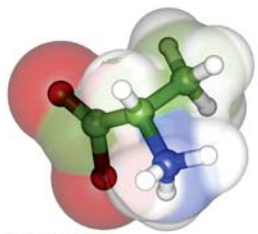

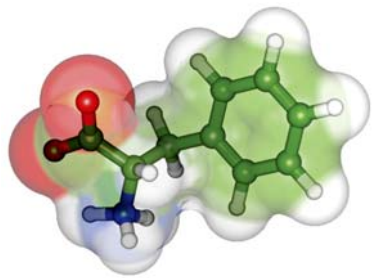

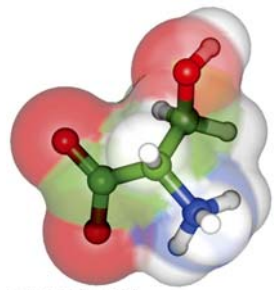

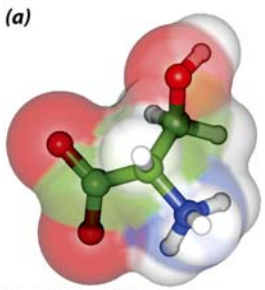

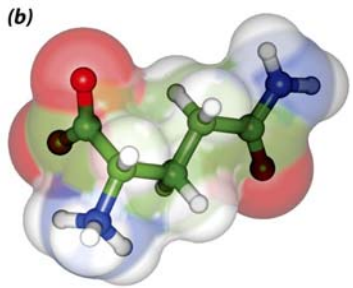

Figure 4-5 Fundamentals of Biochemistry, 2/e
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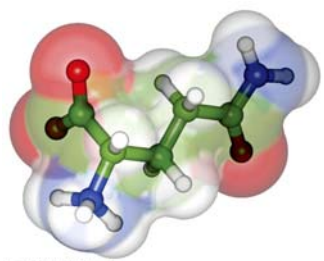

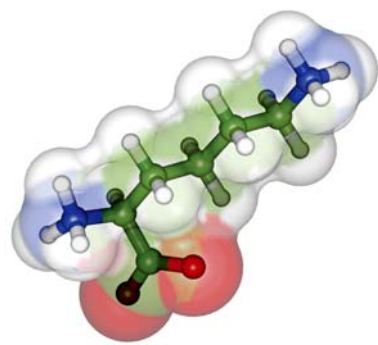

Figure 4-7b Fundamentals of Biochemistry, 2/e
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Peptide bond

Condensation of the two amino acids
Amino acid residue
Amino terminus (N-terminus)
Carboxyl terminus (C-terminus)

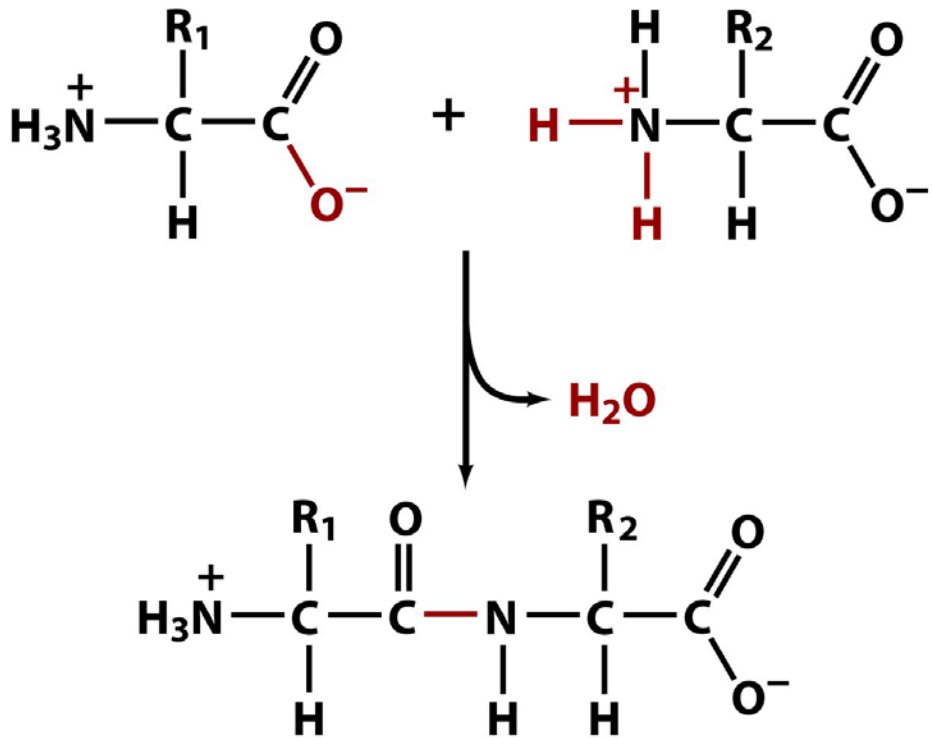


Figure 4-3 Fundamentals of Biochemistry, 2/e

Disulfide bonded cysteine residues

Oxidation and reduction

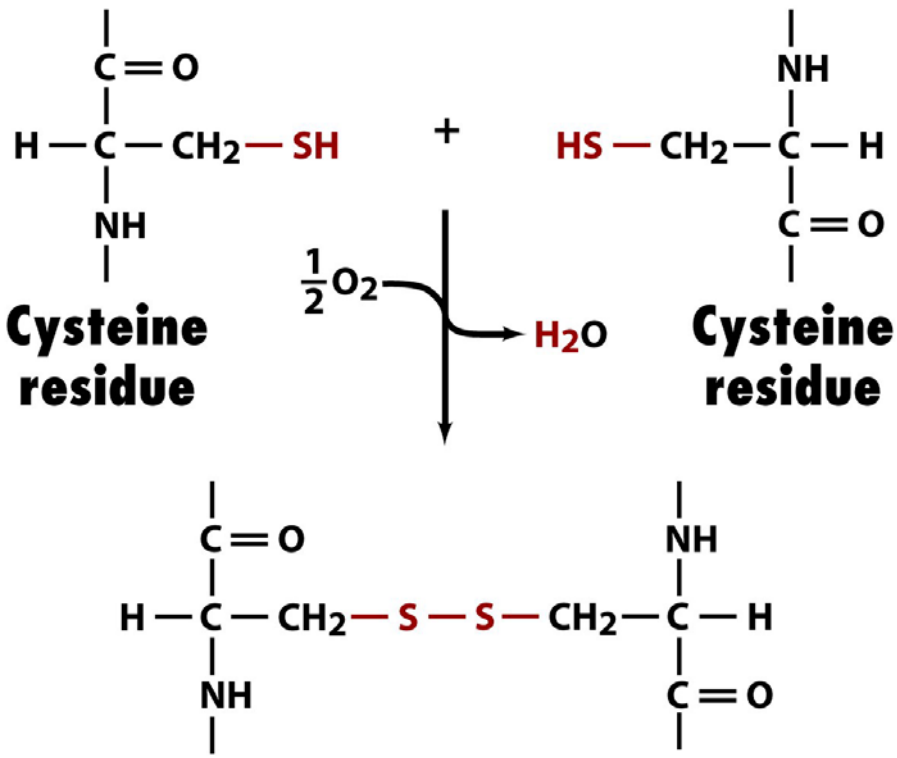


Figure 4-6 Fundamentals of Biochemistry, 2/e

Acid-base properties

pI = isoelectric point
pK values depend on nearby groups

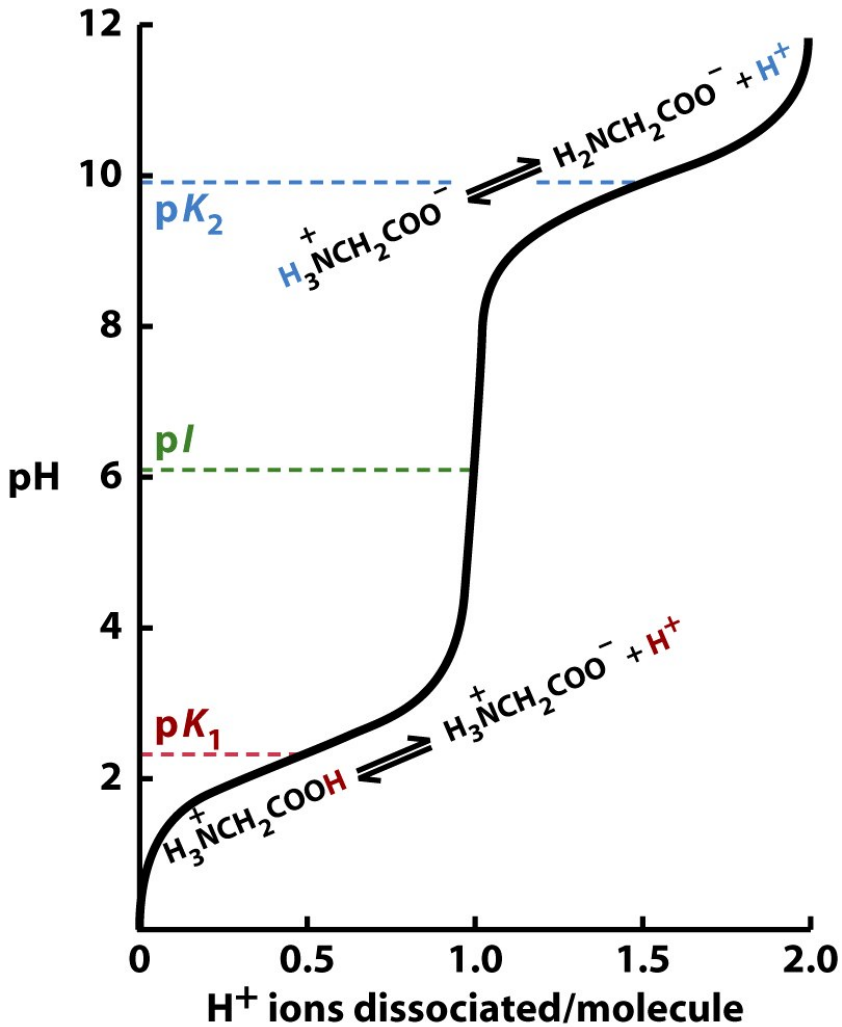


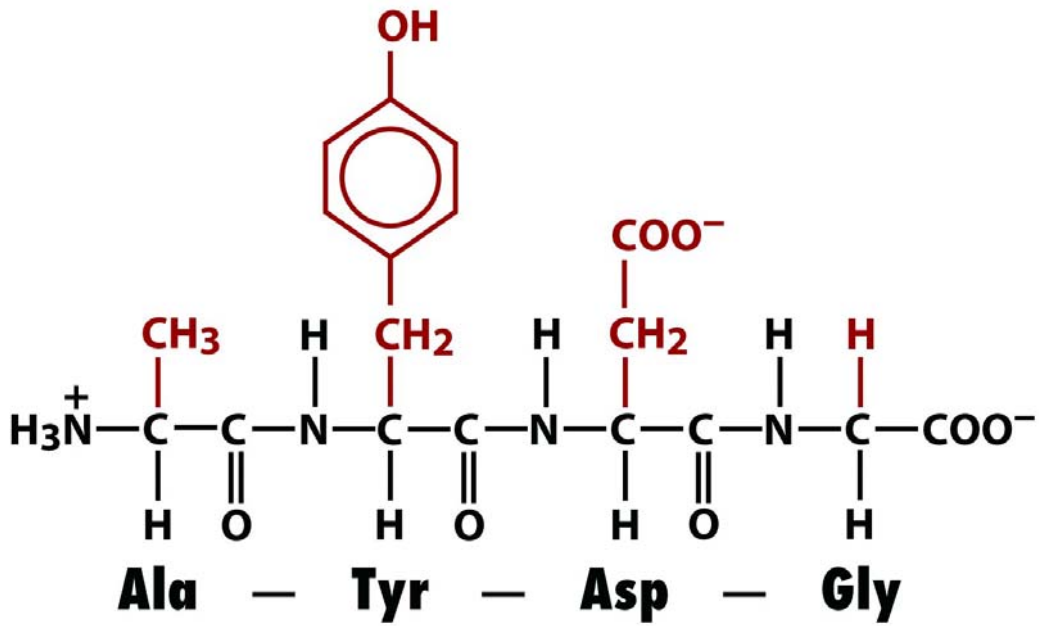
Figure 4-8 Fundamentals of Biochemistry, 2/e

Nomenclature

Alanyltyrosylaspartylglycine

Ala-Tyr-Asp-Gly

AYDG



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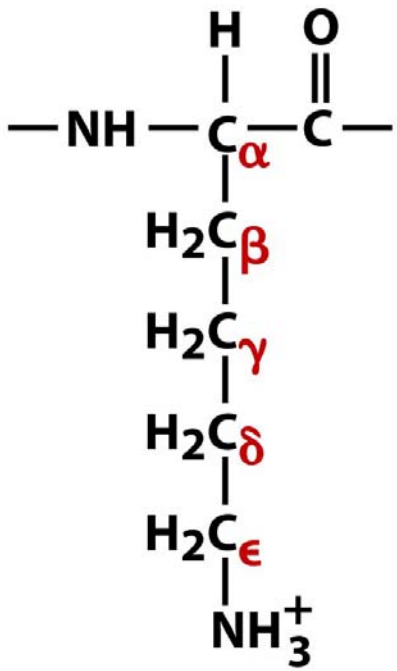
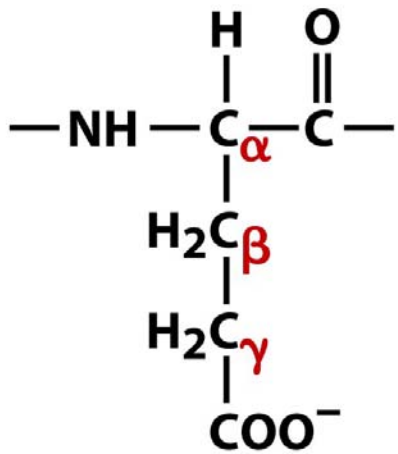
3-letter code

1-letter code



Lys



Glu

Figure 4-9 Fundamentals of Biochemistry, 2/e

Stereochemistry

Optically active molecules are asymmetric

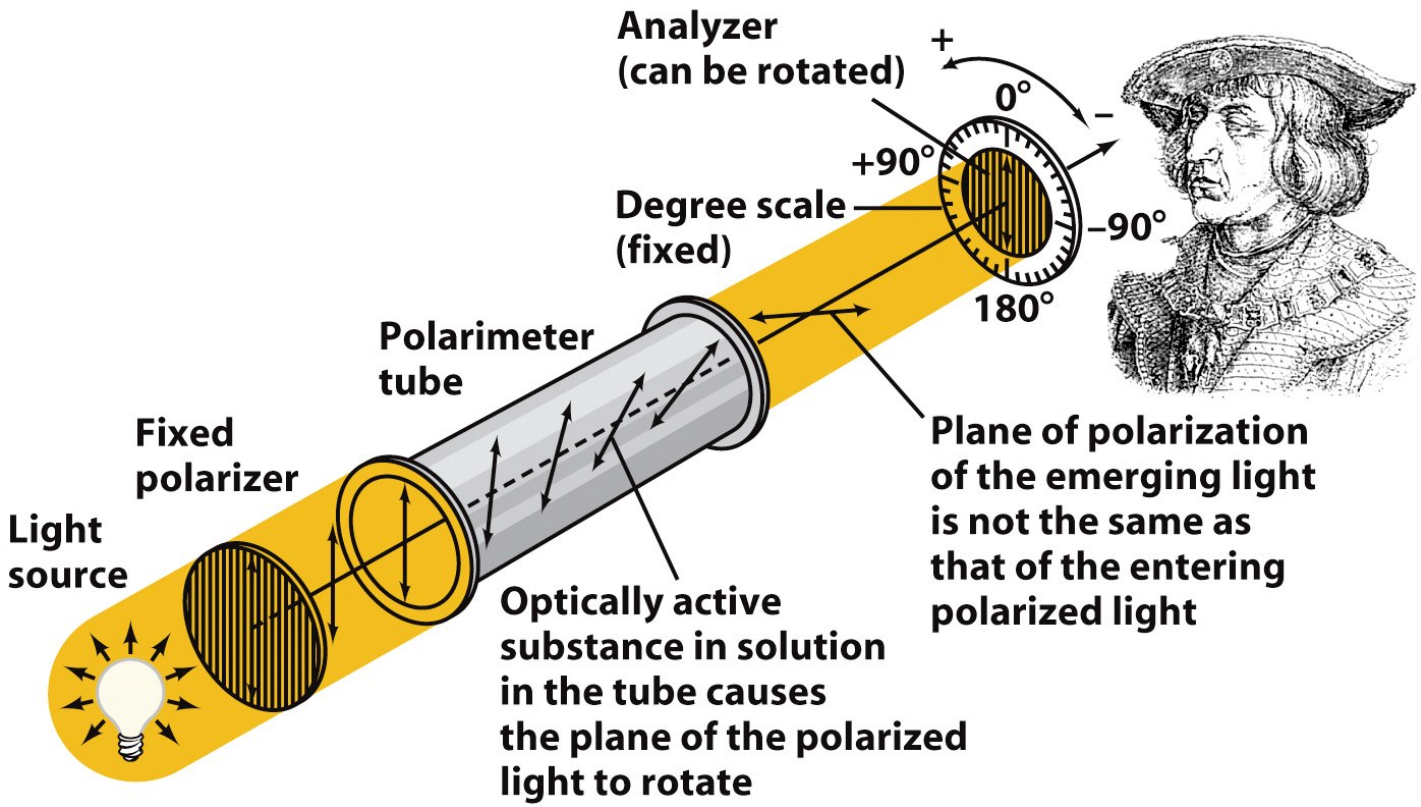


Figure 4-10 Fundamentals of Biochemistry, 2/e

Asymmetric carbon
Asymmetric center
Chiral center
Chirality

Chiral centers give rise to enantiomers

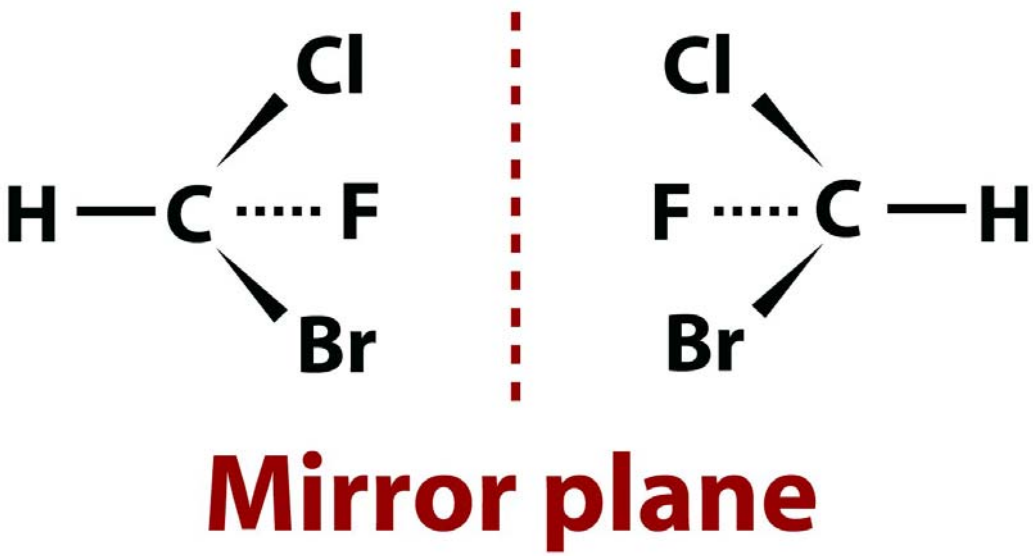


Figure 4-11 Fundamentals of Biochemistry, 2/e

이성질체: 분자식은 같으나 구조 (성질)가 다를 경우 이성질체 (isomer)라 부른다. 성질(물리/화학/광학)

구조이성질체 (constitutional isomer)- 원자가 다르게 연결되어 있을 때
(공유결합의 변형이 없이는 동일한 구조를 가질 수 없다)
ex. n-propanol, iso-propanol

형태이성질체 (이형태체, conformational isomer, confomer)- 형태 (conformation)란 단일결합을 축으로 회전할 때 원자의 배열이 달라지는 것을 말한다.
ex. 에탄의 형태 (eclipsed, staggered)

입체이성질체 (stereoisomer: cis-trans isomer, enantiomer, diastereoisomer, epimer)- 삼차원적인 공간배향이 다른 화합물을 가리킨다.

Enantiomer: nonsuperimposable mirror image

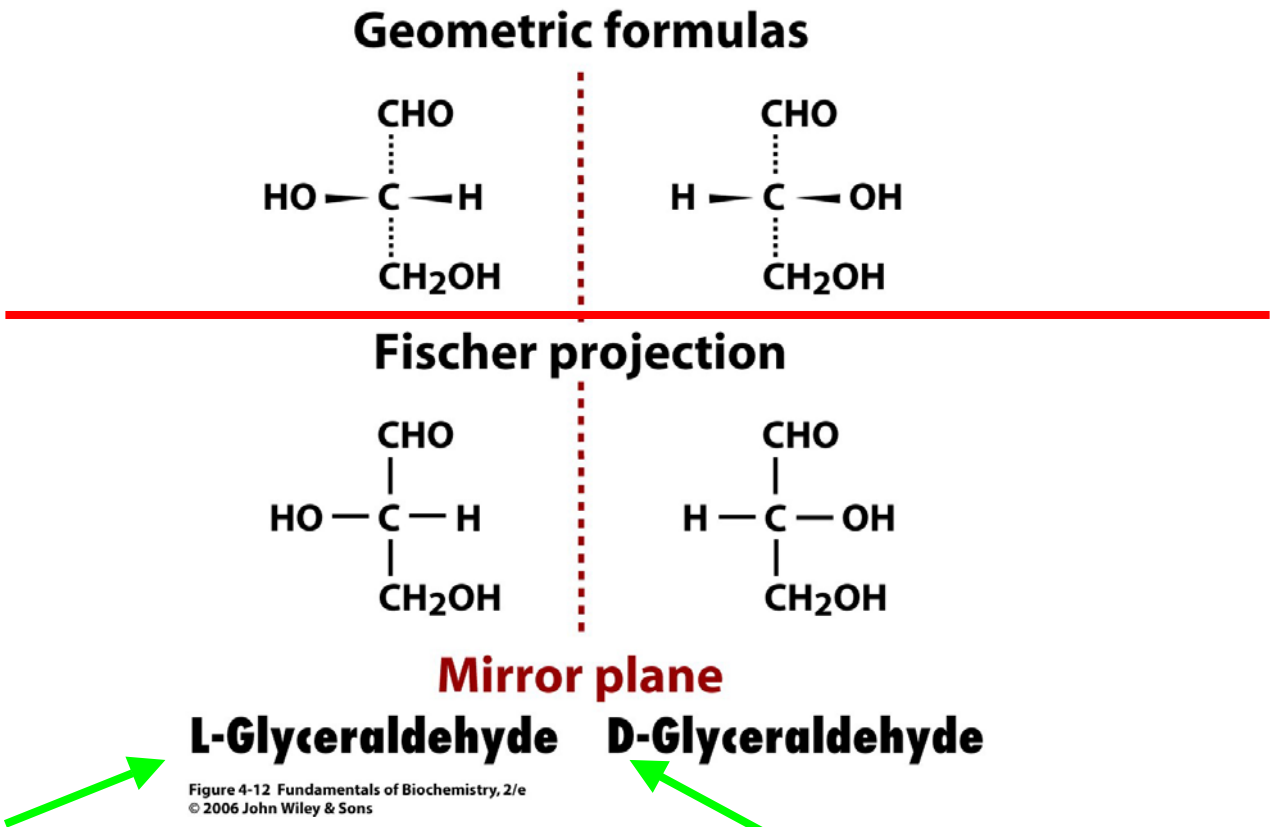
Diastereomer: partial enantiomer

Epimer: isomer that differs at a single chiral center

Configuration & conformation

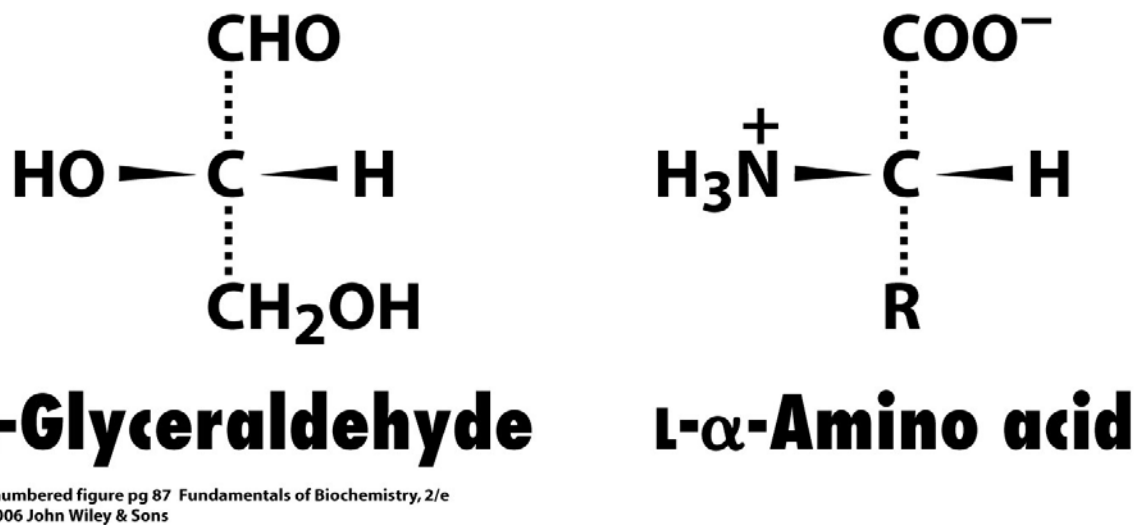
Relative configuration: D/L configuration
Absolute configuration: R/S configuration

The enantiomers of glyceraldehyde



Levorotatory (left)

Dextrorotatory (right)



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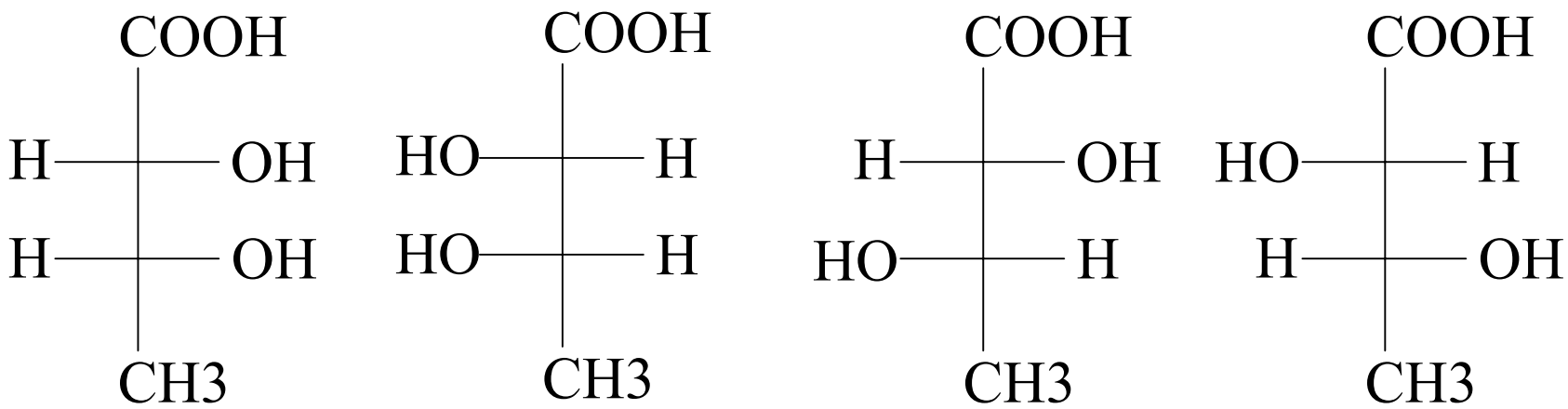
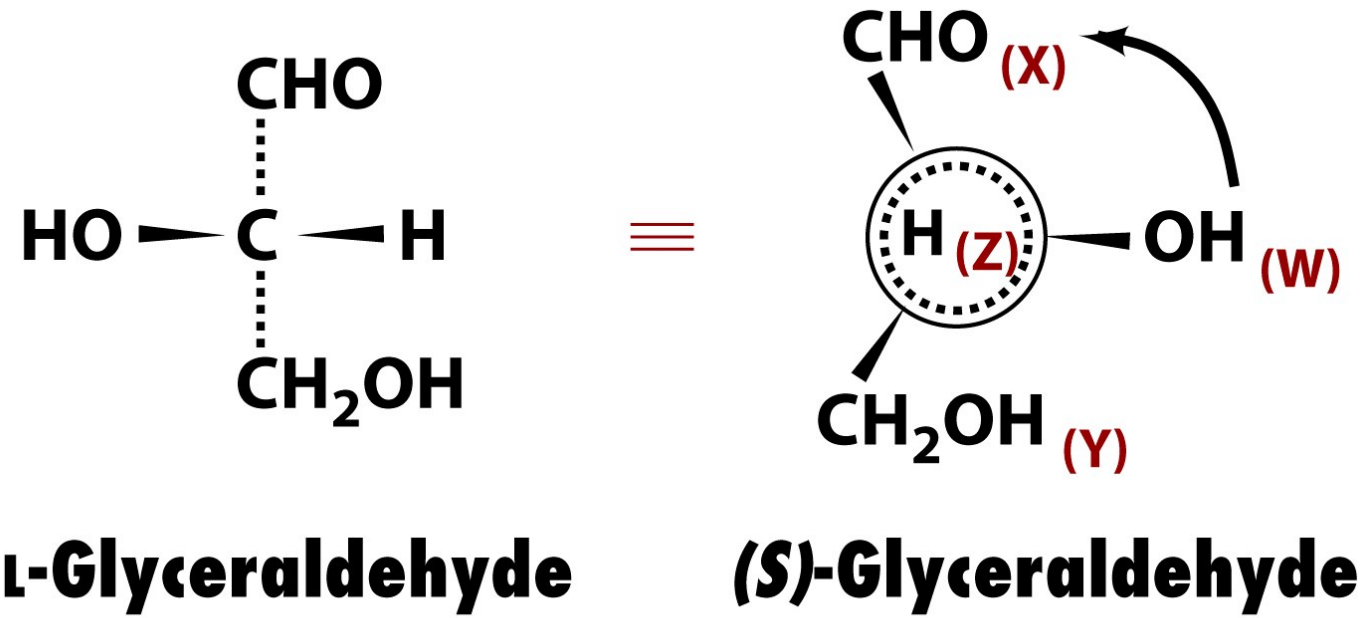
D- and L- in amino acids do not indicate its ability to rotate the plane of polarized light

Absolute configuration: R/S configuration





L-Glyceraldehyde ≡ **(*S*)-Glyceraldehyde**

Box 4-2 Fundamentals of Biochemistry, 2/e

Priority order

The importance of stereochemistry

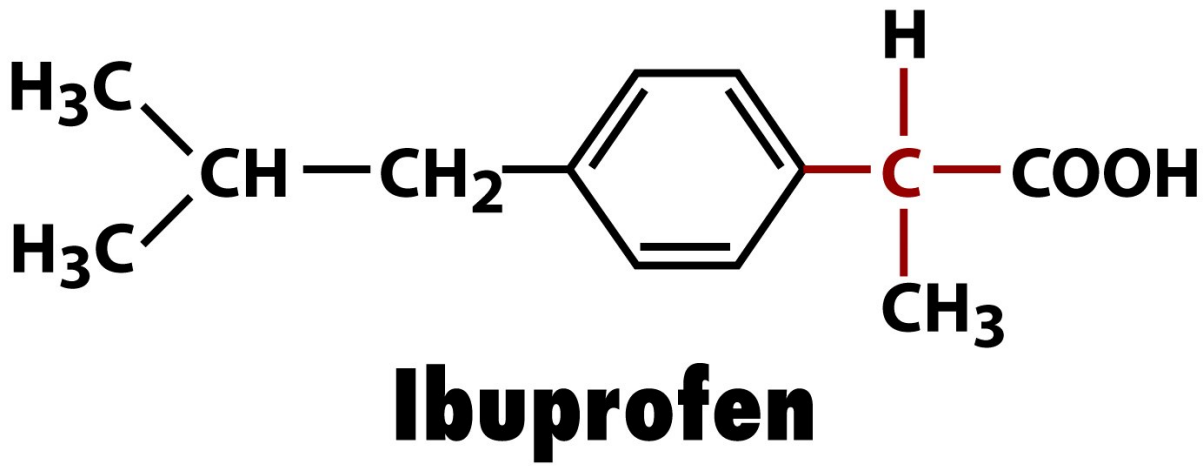
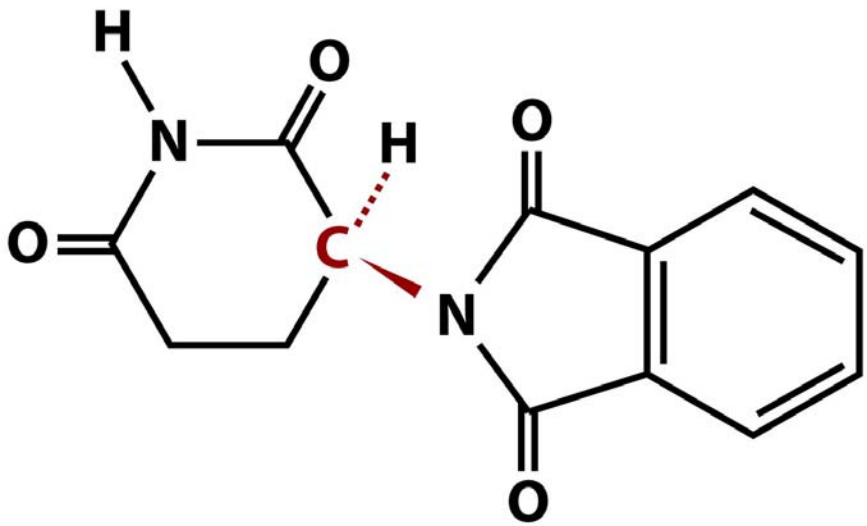


Figure 4-13 Fundamentals of Biochemistry, 2/e



Thalidomide

Figure 4-14 Fundamentals of Biochemistry, 2/e

Its enantiomer causes severe birth defects in human

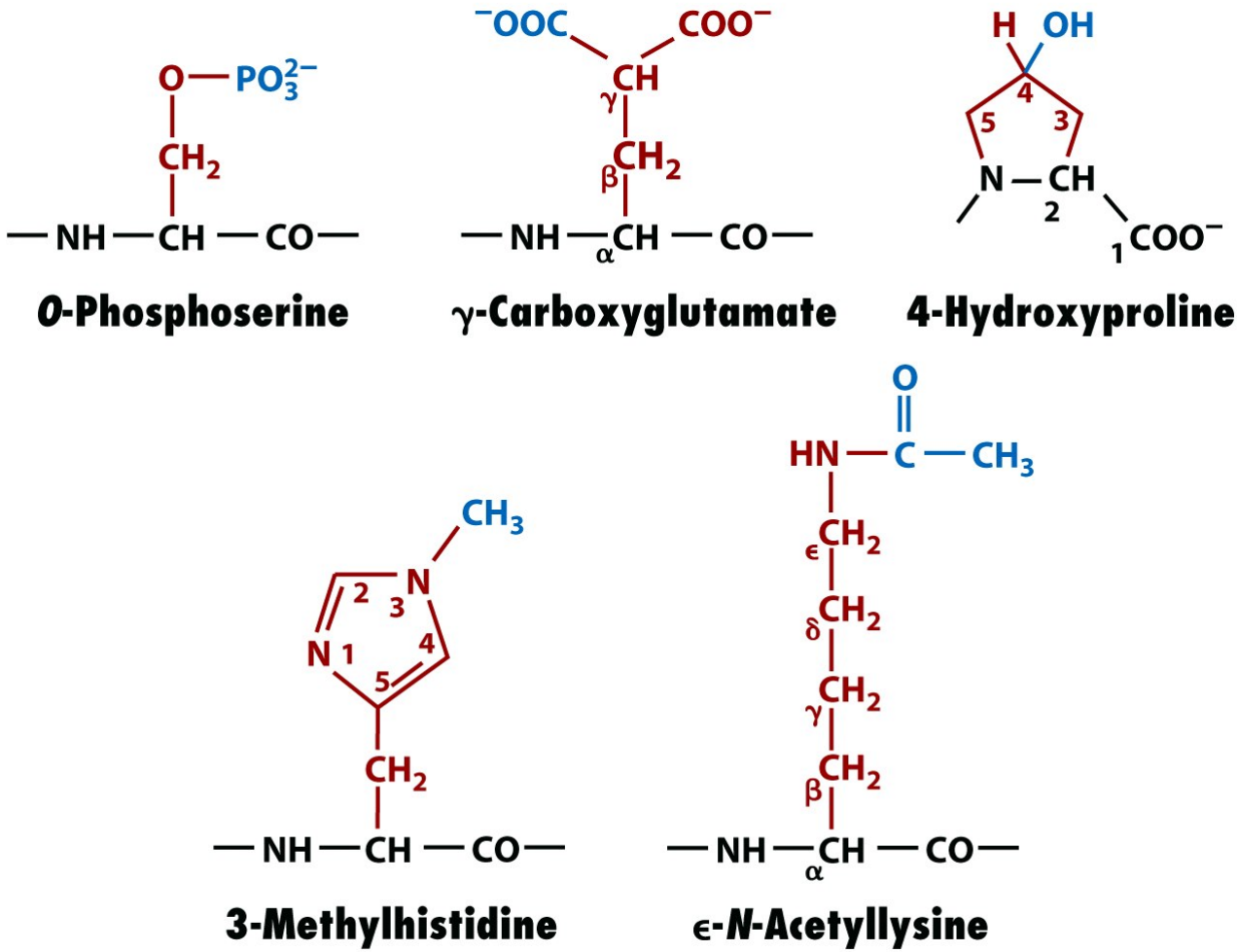
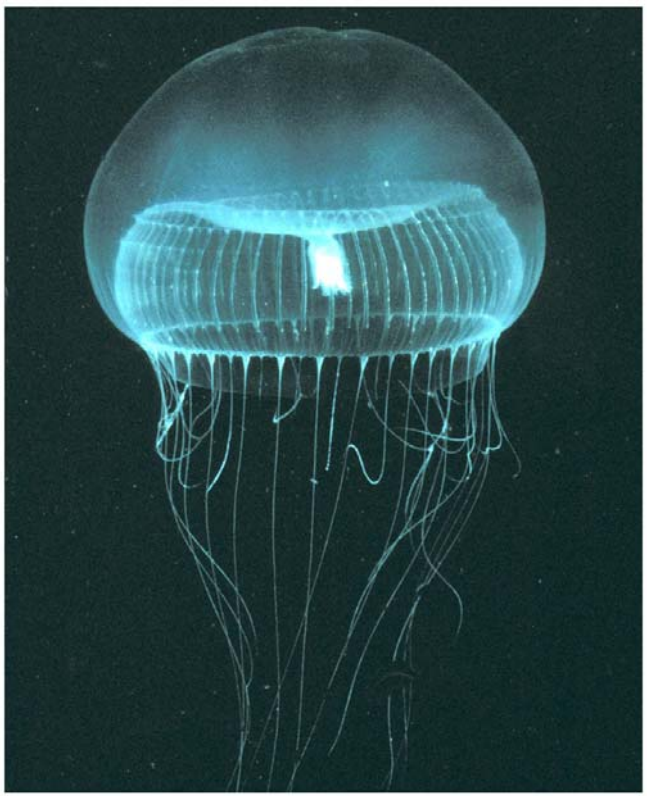
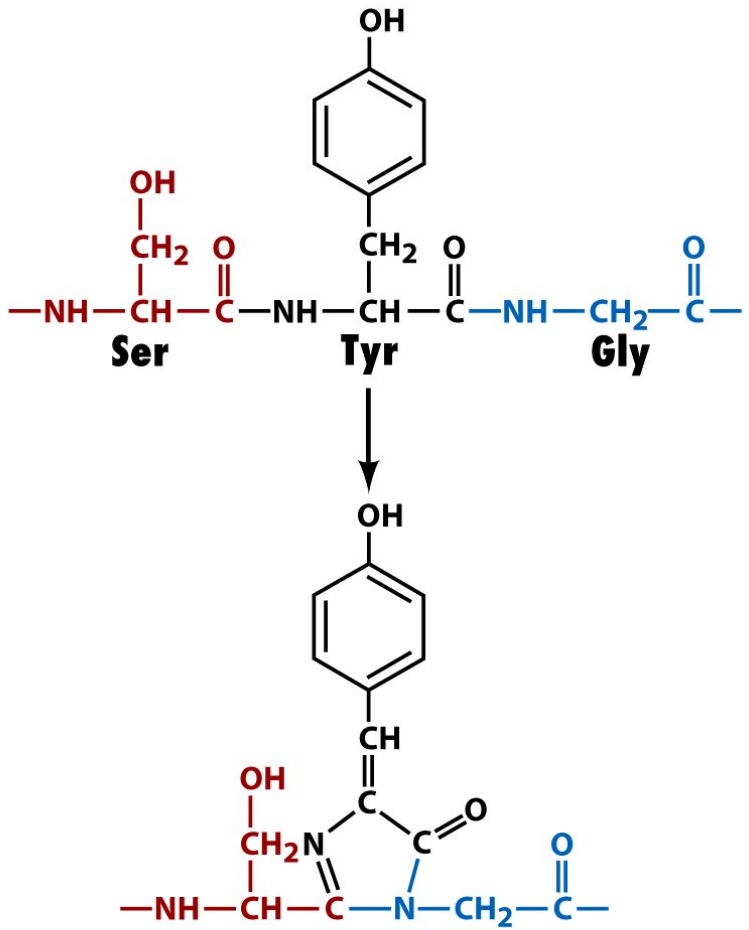


Figure 4-15 Fundamentals of Biochemistry, 2/e



Box 4-3 figure 1 Fundamentals of Biochemistry, 2/e



Fluorophore of green fluorescent protein

Box 4-3 figure 2 Fundamentals of Biochemistry, 2/e

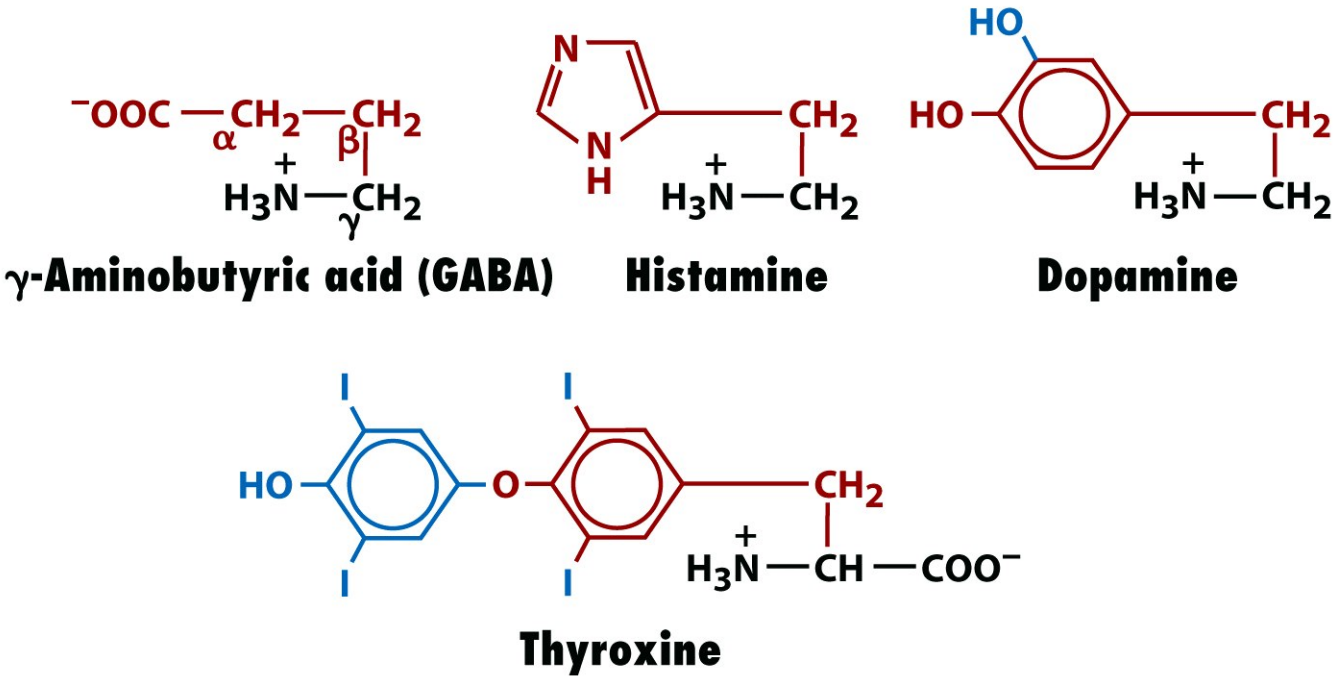
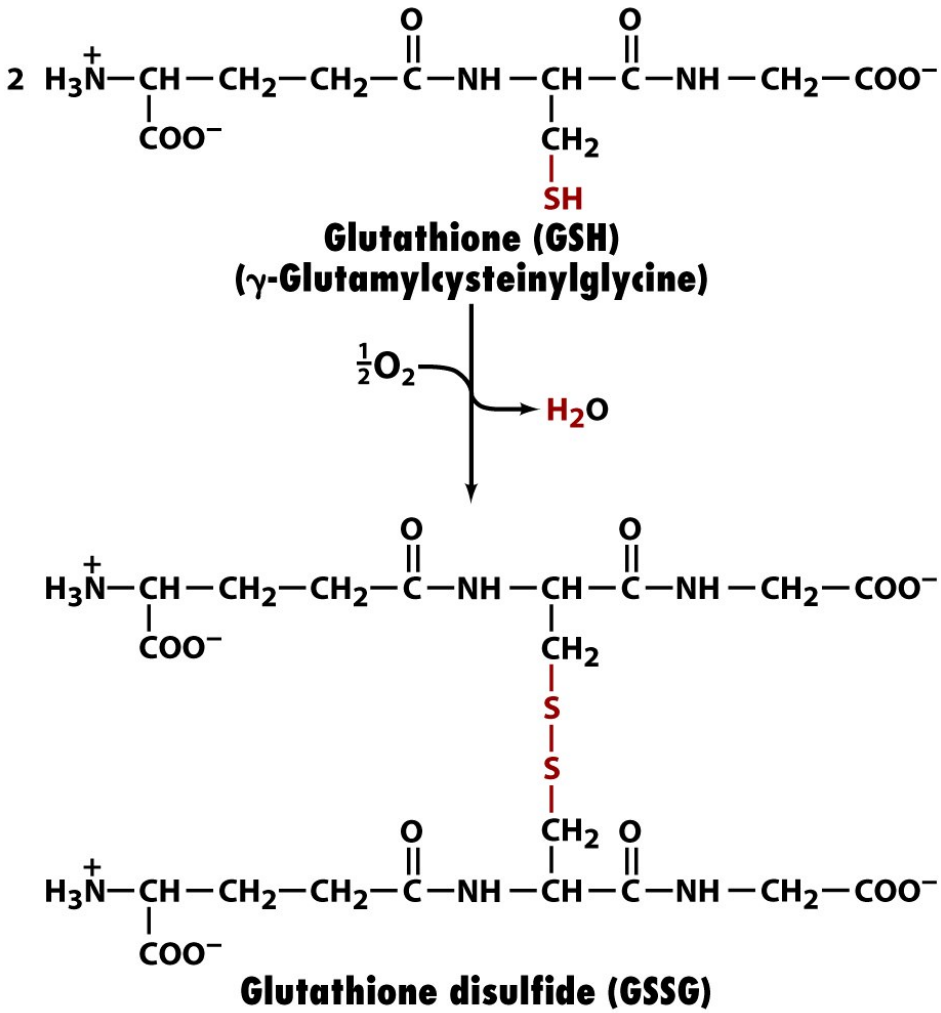


Figure 4-16 Fundamentals of Biochemistry, 2/e



Unnumbered figure pg 91 Fundamentals of Biochemistry, 2/e