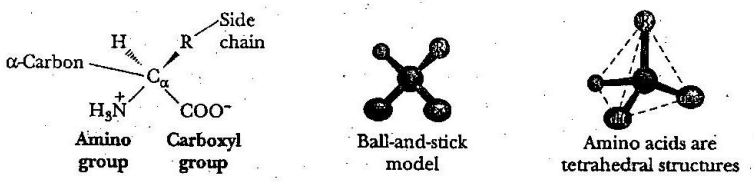
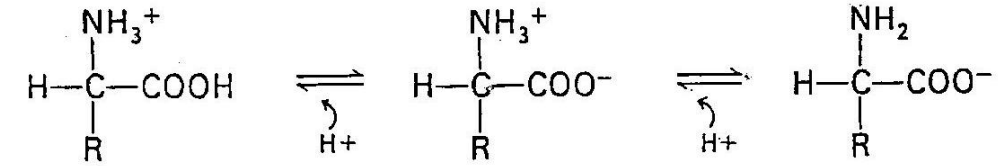
Aminokisline



Anatomy of an amino acid. Except for proline and its derivatives, all of the amino acids commonly found in proteins possess this type of structure.



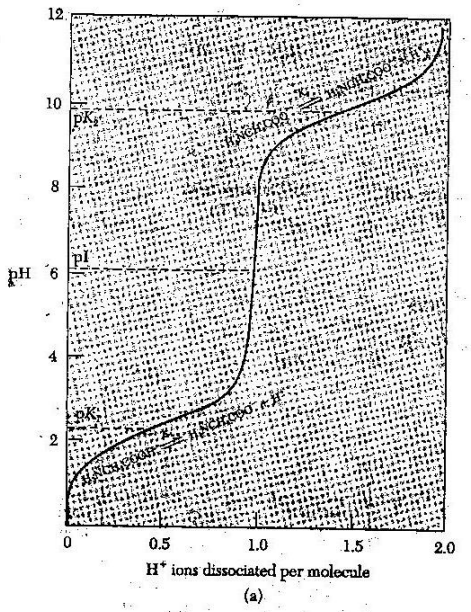
Predominant form at pH 1 | **Predominant form at pH 7** | **Predominant form at pH 11**

amfolit = kislina in baza hkrati
cviter ion (zwitter ion) = dipolarni ion

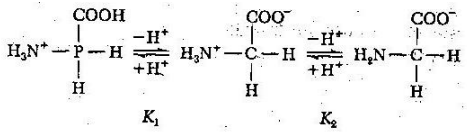
večina ak ~ 300°C

Physical Properties of Some Small Organic Amines and Carboxylic Acids.

Compound	Structural Formula	Molecular Mass (Da)	Melting Point (°C)	Boiling Point (°C)
Ethanoic acid	CH_3COOH	60.05	16.7	118
Propanoic acid	CH_3CH_2COOH	74.08	−21.5	141.1
Butanoic acid	$CH_3CH_2CH_2COOH$	88.1	−7.9	163.5
1-Aminoethane	$CH_3CH_2NH_2$	45.08	−80	16.6
1-Aminopropane	$CH_3CH_2CH_2NH_2$	59.11	−83	48
1-Aminobutane	$CH_3(CH_2)_3NH_2$	73.14	−50	78



(a)



Titration Curve for Glycine. (a) Glycine, a monocarboxylic acid and monoamino amino acid, has two dissociation constants, K_1 and K_2. (b) The equation for glycine dissociation. The dissociation constants, K_1 and K_2, correspond to the loss of the proton from the carboxyl group and the amino group, respectively. The titration curve has two distinct stages. The values of K_1 and K_2 are obtained from the midpoints of the first and second stages, respectively. (*a*, Redrawn from Meister, A., Biochemistry of Amino Acids (2nd ed.), vol. 1, p. 30, 1965, Academic Press,)

$$pH = pK + \log\left(\frac{[A^-]}{[HA]}\right)$$ Henderson-Hasselbalch

$$pI = \frac{1}{2}(pK_i + pK_j')$$

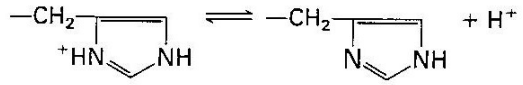
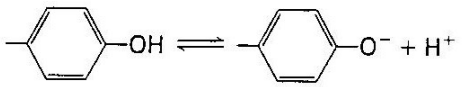
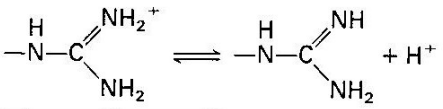
	pKa
CH_3COOH	4.76
alifatski amini	~10.7

Table 4.1

pK Values of Common Amino Acids

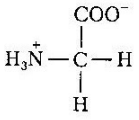
Amino Acid	α-COOH pK_a	α-NH_3^+ pK_a	R group pK_a
Alanine	2.4	9.7	
Arginine	2.2	9.0	12.5
Asparagine	2.0	8.8	
Aspartic acid	2.1	9.8	3.9
Cysteine	1.7	10.8	8.3
Glutamic acid	2.2	9.7	4.3
Glutamine	2.2	9.1	
Glycine	2.3	9.6	
Histidine	1.8	9.2	6.0
Isoleucine	2.4	9.7	
Leucine	2.4	9.6	
Lysine	2.2	9.0	10.5
Methionine	2.3	9.2	
Phenylalanine	1.8	9.1	
Proline	2.1	10.6	
Serine	2.2	9.2	~13
Threonine	2.6	10.4	~13
Tryptophan	2.4	9.4	
Tyrosine	2.2	9.1	10.1
Valine	2.3	9.6	

pK values of ionizable groups in proteins

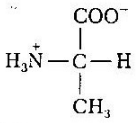
Group	*Acid* $\rightleftharpoons$ *base* + H^+	*Typical* pK*
Terminal carboxyl	$-COOH \rightleftharpoons -COO^- + H^+$	3.1
Aspartic and glutamic acid	$-COOH \rightleftharpoons -COO^- + H^+$	4.4
Histidine		6.5
Terminal amino	$-NH_3^+ \rightleftharpoons -NH_2 + H^+$	8.0
Cysteine	$-SH \rightleftharpoons -S^- + H^+$	8.5
Tyrosine		10.0
Lysine	$-NH_3^+ \rightleftharpoons -NH_2 + H^+$	10.0
Arginine		12.0

*pK values depend on temperature, ionic strength, and the microenvironment of the ionizable group.

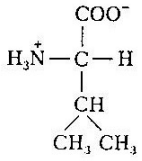
Amino Acids with Nonpolar Side Chains.



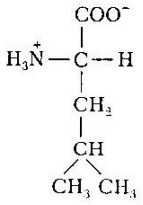
(a) Glycine (Gly or G)



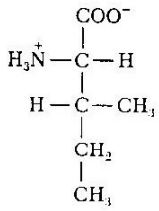
(b) Alanine (Ala or A)



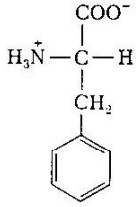
(c) Valine (Val or V)



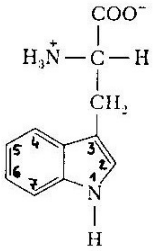
(d) Leucine (Leu or L)



(e) Isoleucine (Ile or I)

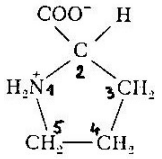


(f) Phenylalanine (Phe or F)



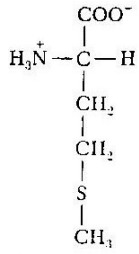
(g) Tryptophan (Trp or W)

R = indolna s.



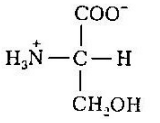
(h) Proline (Pro or P)

R = pirolidinska s.

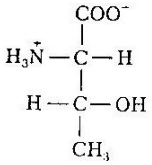


(i) Methionine (Met or M)

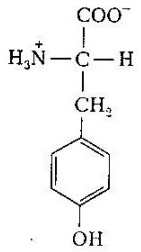
Amino Acids with Polar but Uncharged Side Chains.



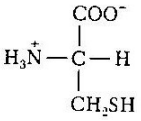
(a) Serine (Ser or S)



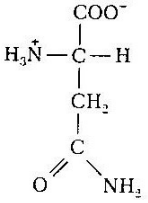
(b) Threonine (Thr or T)



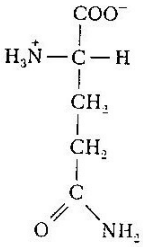
(c) Tyrosine (Tyr or Y)



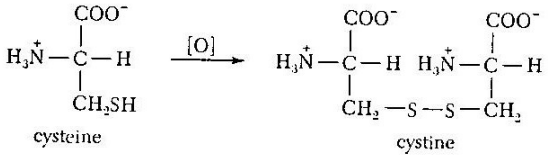
(d) Cysteine (Cys or C)



(e) Asparagine (Asn or N)



(f) Glutamine (Gln or Q)

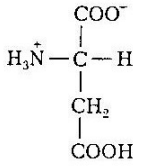


cysteine

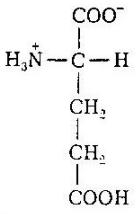
cystine

Oxidation of Cysteine to Form Cystine.

Amino Acids with Acidic Side Chains.

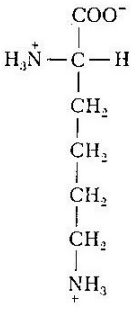


(a) Aspartic acid
(Asp or D)

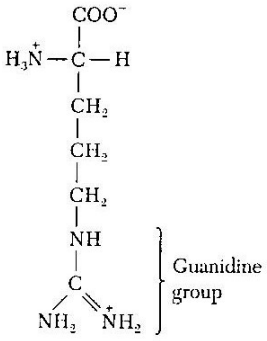


(b) Glutamic acid
(Glu or E)

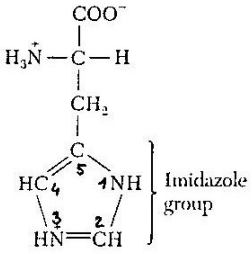
Amino Acids with Basic Side Chains.



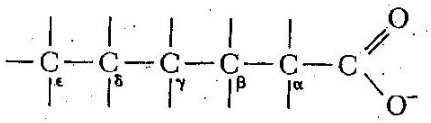
(a) Lysine
(Lys or K)



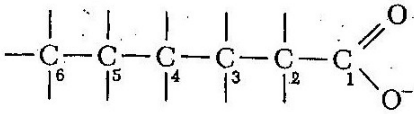
(b) Arginine
(Arg or R)



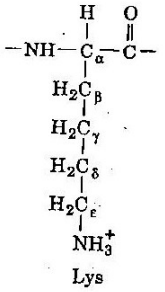
(c) Histidine
(His or H)



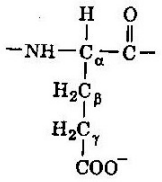
Pre-IUPAC nomenclature system



IUPAC nomenclature system



Lys

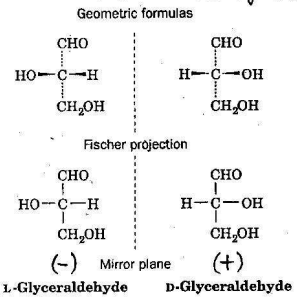


Glu

Razen Gly so vse ak optično aktivne.
asimetrični ali kiralni center (kiralnost)
enantiomera, diastereomera
specifična rotacija $[\alpha]_D^{25}$ → +, −
(Na D črta (589.3 nm))
\+ dekstrorotatorna (d)
− levorotatorna (l)

Relativna konfiguracija

1891: E. Fischer : določitev relat. konf. (+)Glc (Nobelova 1902)

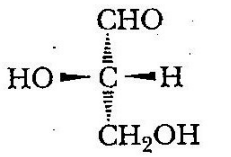


The Fischer convention configurations for naming the enantiomers of glyceraldehyde as represented by geometric formulas (*top*) and their corresponding Fischer projection formulas (*bottom*). Note that in Fischer projection, all horizontal bonds point above the page and all vertical bonds point below the page. The mirror planes relating the enantiomers are represented by a vertical dashed line. (Fischer projection formulas, as traditionally presented, omit the central C symbolizing the chiral carbon atom. The Fischer projection formulas in this text, however, will generally have a central C.)

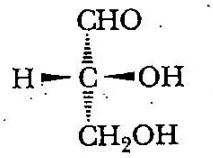
1906 : Rossanoff, M. (Fischerjeva konvencija)
(+)gliceraldehid → D-gliceraldehid
(−)gliceraldehid → L-gliceraldehid

1951 : X-žarkovna kristalografija (Bijvoet, J.M.)
relativna ≡ **absolutna** konfiguracija

gliceraldehid	α-ak
-OH →	$-NH_3^+$
-CHO →	-COOH
$-CH_2OH$ →	-R
-H →	-H

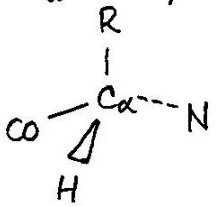


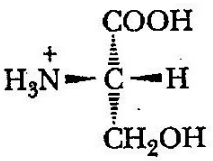
L-Glyceraldehyde



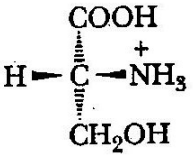
D-Glyceraldehyde

"CORN" pravilo:
pomoč pri razvrstitvi skupin okoli C_α atoma pri L-α-ak!





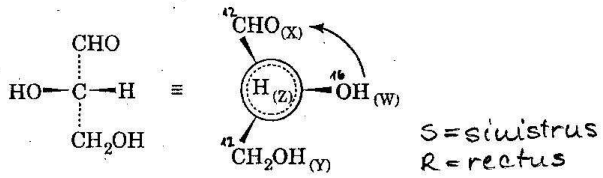
L-Serine



D-Serine

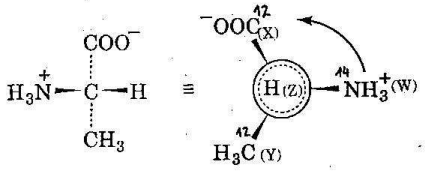
1956: absolutna nomenklaturna shema
Cahn – Ingold – Prelog

Atomi z višjim atom. številom vezani na kiralni center imajo višjo prioriteto



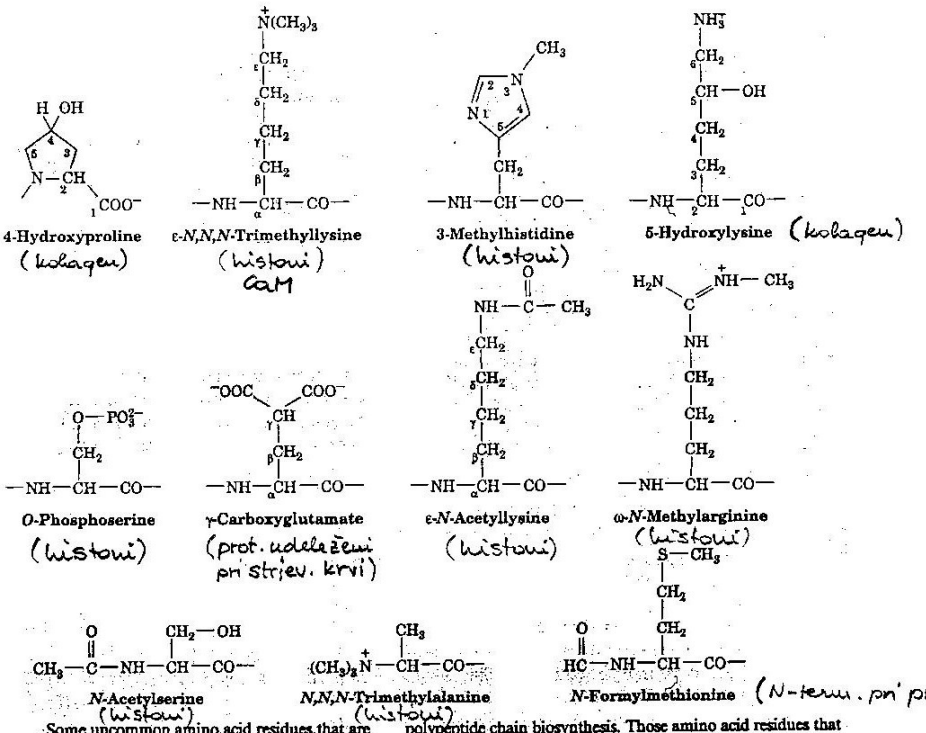
L-Glyceraldehyde **(*S*)-Glyceraldehyde**

The structural formula of L-glyceraldehyde and its equivalent (*RS*)-system representation indicating that it is (*S*)-glyceraldehyde. In the latter drawing, the chiral C atom is represented by the large circle, and the H atom, which is located behind the plane of the paper, is represented by the smaller concentric dashed circle.



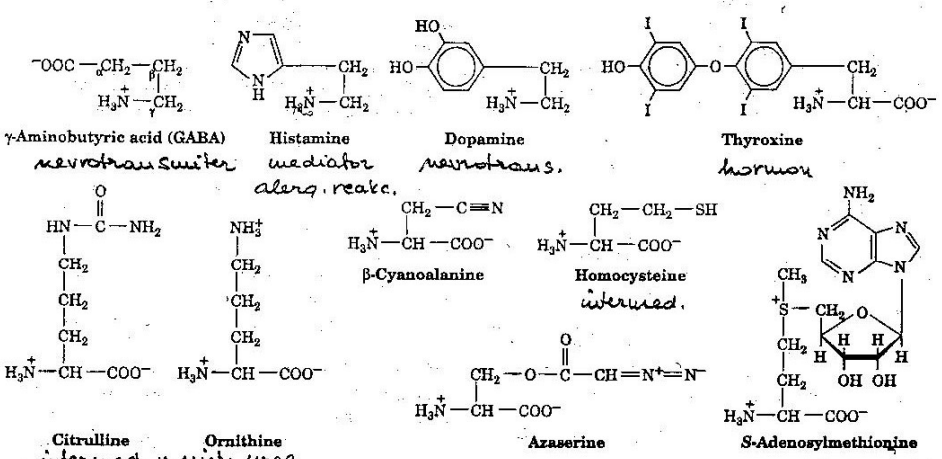
L-Alanine **(*S*)-Alanine**

The structural formula of L-alanine and its equivalent (*RS*)-system representation indicating that it is (*S*)-alanine.



Some uncommon amino acid residues that are components of certain proteins. All of these residues are modified from one of the 20 "standard" amino acids after polypeptide chain biosynthesis. Those amino acid residues that are derivatized at their N_α position occur at the N-termini of proteins.

D-ak : polipeptidi bakt. cel. sten ; bakterijski antibiotiki (valinomicin, gramicidin A ...)



Some biologically produced derivatives of "standard" amino acids and amino acids that are not components of proteins.