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21 L-α-Amino Acids proteins polypeptide isoelectric point IEP protolysis pK_a value

At physiologic pH=7, 36 ±0.01 carboxylic groups **R-COO⁻** negative charged and amino groups **R-NH$_3^+$** positive charged. For example, glutamic acid pK_a reference to physiologic pH value smaller as $pK_{aR\text{-}COO^-}$=4.25<7.36, pK_{aCOO^-}=2.19<7.36 and for amine is greater as physiologic pH: 9.67=$pK_{a\text{-}NH3+}$>7.36 .

Table shown constants pK_a of four type parallel protolytic equilibria in each amino acid molecule:

acid	⇔ base	$+H^+$;
1. **R-COOH**	⇔**R-COO⁻**	$+H^+$;
2. **R-NH$_3^+$**	⇔**R-NH$_2$**	$+H^+$;
3. **Tyr**-phenol-**OH**	⇔**Tyr**-phenol-**O⁻**	$+H^+$,
4. Cys-SH	⇔Cys-**S⁻**	$+H^+$

Parallel protolytic equilibria number NpKa average isoelectric point and constant pK_a value IEP= pK_a is calculated as IEP= pK_a= (Σ $pK_{a\ R\ group}$+ $pK_{a\text{-}NH3+}$+ $pK_{a\text{-}COOH}$)/NpK$_a$

In *Ostwald's dilution law* calculate pH of solution at concentration C logarithm: $pH=\frac{pK_a - \log C}{2}$ =.....

Amino acid and protein at isoelectric point value pH=**IEP** sum of total overall **ion** charge is zero

0—— acidic charge (+)————zero „**0**" charge **IEP**————in basic medium charge minus (-)——→pH scale

-COOH & **-NH$_3^+$** positive charge .....**-COO⁻** & **-NH$_3^+$**..... charge is negative **-COO⁻** & **-NH$_2$**

http://aris.gusc.lv/ChemFiles/Albumin/1E7GpI.doc !E7G.pdb;IgG1.pdb

http://aris.gusc.lv/ChemFiles/ChromoHem/MyoGlobOxDeoxCoBiliverdin/1MBOaaLin153.doc ! 1MBO.pdb;

Amino Acid	pKa-COOH	pKa-NH3+	pKa R group
Isoleucine	2.36	9.68	
Valine	2.32	9.62	
Leucine	2.36	9.60	
Phenylalanine	1.83	9.13	
Cysteine	1.96	10.28	8.18
Methionine	2.28	9.21	
Alanine	2.34	9.69	
Proline	1.99	10.96	
Glycine	2.34	9.60	
Threonine	2.11	9.62	
Serine	2.21	9.15	
Tryptophan	2.38	9.39	
Tyrosine	2.20	9.11	10.07
Histidine	1.82	9.17	6.00
Aspartate	1.88	9.60	3.65
Glutamate	2.19	9.67	4.25
Asparagine	2.02	8.80	
Glutamine	2.17	9.13	
Lysine	2.18	8.95	10.53
Arginine	2.17	9.04	12.48

Table5.3 Reginald H. Garrett, Charles M. Grishman, **Biochemistry**, University of Virginia 1995

Myoglobin IEP=7,36 is neutral zero „**0**" charged molecule, as IEP=7,36 is equal physiologic pH_{blood}=7,36 1MBO.pdb

Albumin molecule E7G.pdb 7,32=IEP 7 fatty acids small (–) charge and 7,40=IEP absent 7 faaty acids (+) positive at physiologic pH=7.36, but gamma *Globulin* IgG1.pdb molecule has positive (+) charge, as at physiologic pH=7.36 is greater IEP=7.91.

Iso electric point IEP=pK_a as well protolytic constant pK_a calculates one of side residues R constants sum $\Sigma pK_{aRside\ residue}$ plus $pK_{aNterminusNH3+}$ and plus $pK_{aCterminusCOO-}$ sum dividing with number NpKa of acidic groups in molecule IEP=pK_a=($\Sigma pK_{aR\ side\ residue}$+$pK_{aNterminus}$+$pK_{aCterminus}$)/NpKa

Figure Separation of serum proteins by **electrophoresis**. (a) A sample is applied as a narrow line at the origin. After **electrophoresis** at pH **8.8**, the paper is dried and stained. (b) A plot of color intensity of each spot. γ *Globulin* moves slower as *Albumin* .

Proteins move this direction ← spot line position sample origin at start

Positive (+) electrode

Direction of movement

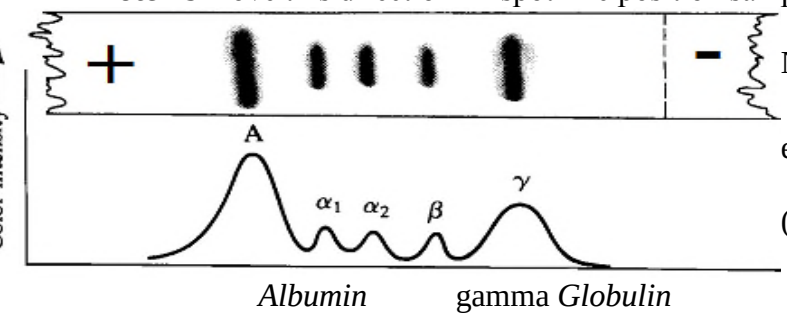
<=————

Albumin

IEP=7,32 << **pH=8,8**

γ *Globulin*

IEP=7,91 < **pH=8,8**



Negative (-) electrode

(a)

(b)

Albumin gamma *Globulin*

Seleno cysteine, the 21st L-α-Amino Acid

Seleno cysteine is an L-α-amino acid found in a handful of proteins, including certain **peroxidases** and **reductases** where it participates in the catalysis of electron transfer reactions.As its name implies, a selenium **Se** atom replaces the sulfur **S** of its structural analog, cysteine. The pK_3 of seleno cysteine 5.2 is 3 units lower than that of cysteine 8.18. Since seleno cysteine is inserted into polypeptides during translation, it is commonly referred to as the "21st amino acid." However, like the other 20 genetically encoded amino acids, seleno cysteine is specified by a simple three-letter codon **UGA** (see class 16 week Nucleo proteins tRNA 62 codons).

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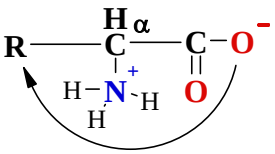
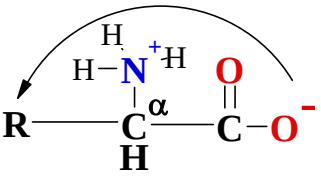
Draw fisher projections for 3D molecules Harper's Biochemistry tab1e-3 on 15-16 page wrong D- to L-α-amino acids to fill table right side:http://aris.gusc.lv/06Daugavpils/Research/Amineac20L.doc, as L-α-amino acids! Santa Barbarbara University 3D molecules:http://aris.gusc.lv/ChemFiles/MCDB108A/tw-amn/aasframes.htm.

Harper's Biochemistry Illustrated Table 3-1 shows D-amino acids Fisher projections, which are wrong for human organism proteins. Your task is in **Table** right side to show L-α-amino acids



CW Clock Wise

L-α-amino acids Fisher projections
CCW Counter Clock Wise
Levos rotational



L-α-amino acids Fisher projections CCW Counter Clock

Table The 20 common L-α-amino acids found in protein. Physiologic pH=7.36 .

Protein-derived Amino Acids with **aliphatic** side chains left side	**Name**	**Symbol**	**Show Fisher projection Structural Formula**
1	Glycine	Gly [G]	
2	Alanine	Ala [A]	
3	Valine	Val [V]	
4	Leucine	Leu [L]	
5	Isoleucine	Ile [I]	
With side chains containing **hydroxyl (—OH)** groups left side			
6	Serine	Ser [S]	
7	Threonine	Thr [T]	
18	Tyrosine	Tyr [Y]	Show below ↓.
With side chains containing **Sulfur** atoms **(—S— ; —SH)** left side			
8	Cysteine	Cys [C]	
9	Methionine	Met [M]	

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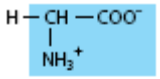
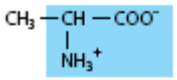
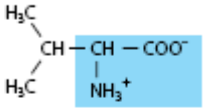
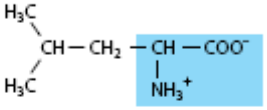
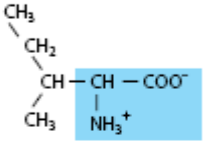
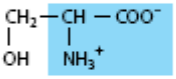
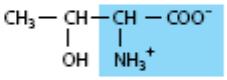
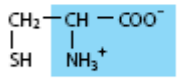
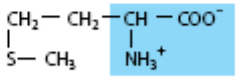
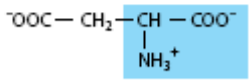
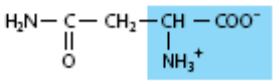
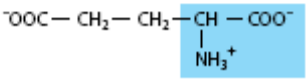
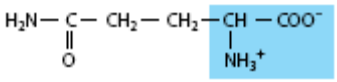
Table The 20 common L-α-amino acids found in protein. . Physiologic pH=7.36 .

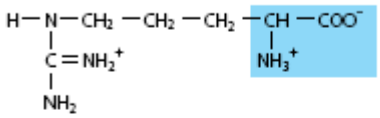
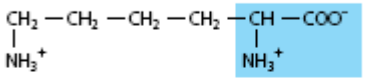
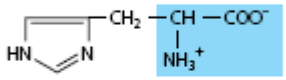
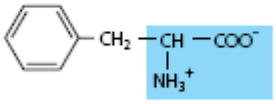
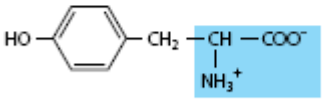
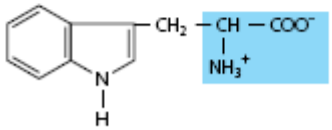
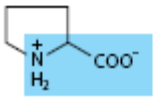
	Name	Symbol	Show Fisher projection Structural Formula
With side chains containing **Acidic (—COO⁻)** groups or their **Amides (—CO—NH$_2$)**			
left side 10	Aspartate Aspartic acid salt	Asp [D]	
11	Asparagine	Asn [N]	
12	Glutamate Glutamic acid salt	Glu [E]	
13	Glutamine	Gln [Q]	
With side chains containing **Basic (—NH$_n^{(+)}$) Groups**			
left side 14	Arginin	Arg [R]	
15	Lysine	Lys [K]	
16	Histidine	His [H]	
Containing **Aromatic** Rings 16 left side	Histidine	His [H]	Show above ↑
17	Phenylalanine	Phe [F]	
18	Tyrosine	Tyr [Y]	
19	Tryptophan	Trp [W]	
Imino Acid			
20	Proline	Pro [P]	

Table 3–1. L-α-Amino acids present in proteins.

Name	Symbol	Structural Formula	pK_1 α-COOH	pK_2 α-NH_3^+	pK_3 R Group
With Aliphatic Side Chains					
Glycine	Gly [G]		2.4	9.8	
Alanine	Ala [A]		2.4	9.9	
Valine	Val [V]		2.2	9.7	
Leucine	Leu [L]		2.3	9.7	
Isoleucine	Ile [I]		2.3	9.8	
With Side Chains Containing Hydroxylic (OH) Groups					
Serine	Ser [S]		2.2	9.2	about 13
Threonine	Thr [T]		2.1	9.1	about 13
Tyrosine	Tyr [Y]	See below.			
With Side Chains Containing Sulfur Atoms					
Cysteine	Cys [C]		1.9	10.8	8.3
Methionine	Met [M]		2.1	9.3	
With Side Chains Containing Acidic Groups or Their Amides					
Aspartic acid	Asp [D]		2.0	9.9	3.9
Asparagine	Asn [N]		2.1	8.8	
Glutamic acid	Glu [E]		2.1	9.5	4.1
Glutamine	Gln [Q]		2.2	9.1	

(continued)

Table 3–1. L-α-Amino acids present in proteins. (continued)

Name	Symbol	Structural Formula	pK_1	pK_2	pK_3
With Side Chains Containing Basic Groups			α-COOH	α-NH_3^+	R Group
Arginine	Arg [R]		1.8	9.0	12.5
Lysine	Lys [K]		2.2	9.2	10.8
Histidine	His [H]		1.8	9.3	6.0
Containing Aromatic Rings					
Histidine	His [H]	See above.			
Phenylalanine	Phe [F]		2.2	9.2	
Tyrosine	Tyr [Y]		2.2	9.1	10.1
Tryptophan	Trp [W]		2.4	9.4	
Imino Acid					
Proline	Pro [P]		2.0	10.6	