IUPAC – PREPORUKE IMENOVANJA I GRAFIČKOG PRIKAZIVANJA U PEPTIDNOJ KEMIJI

IUPAC – RECOMMENDATIONS FOR NOMENCLATURE AND GRAPHICAL REPRESENTATION IN PEPTIDE CHEMISTRY

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International Union for Pure and Applied Chemistry

Međunarodna unija za čistu i primijenjenu kemiju

1911. Pariz, inicijativa Međunarodnog udruženja kemijskih društava (IACS), potreba za djelovanjem i rješavanjem problema u kemiji

28. srpnja 1919. utemeljenje IUPAC-a

1919 – 2019. IUPAC prerasta u međunarodno priznato autoritativno tijelo u području:

- nomenklature anorganskih i organskih spojeva
- nazivlja u kemiji
- imenovanja novih elemenata u periodnom sustavu elemenata
- normiranja mjernih metoda
- normiranja fizikalnih konstanti....

International Union for Pure and Applied Chemistry

Međunarodna unija za čistu i primijenjenu kemiju

Organizacijska struktura IUPAC-a podijeljena u osam odjela

- **Odjel za kemijsku nomenklaturu i prikaz struktura**

  (engl. *Division for Chemical Nomenclature and Structure Representation*)

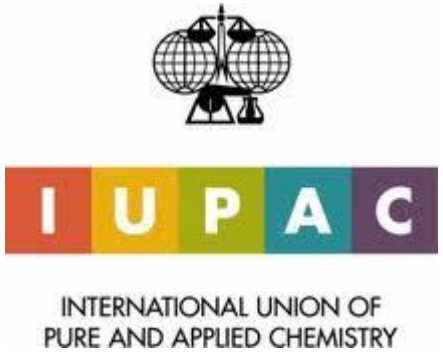
- **Odjel za polimere** (engl. *Polymer Division*)

  Podkomisija za terminologiju polimera (engl. *Subcommittee on Polymer Terminology*)

Međuodjelni odbor za terminologiju, nomenklaturu i simbole
(engl. *Interdivisional Committee on Terminology, Nomenclature and Symbols*, ICTNS)

↓

IUPAC-ove preporuke



(1919. god.)

INTERNATIONAL UNION OF BIOCHEMISTRY AND MOLECULAR BIOLOGY

(1955. god.)

IUPAC-IUBMB *Joint Commission on Biochemical Nomenclature* (JCBN) **(1977. god.)**

Nomenclature Committee of IUBMB (NC-IUBMB)

IUPAC – objave preporuka za nomenklaturu i terminologiju

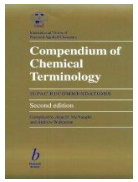
Časopisi

Pure and Applied Chemistry (PAC)
https://www.degruyter.com/view/j/pac

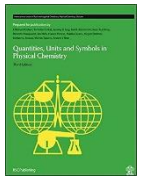
European Journal of Biochemistry/ The FEBS Journal
https://febs.onlinelibrary.wiley.com

Knjige

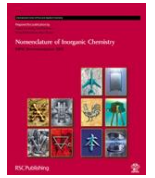
Gold Book Chemical Terminology (Gold Book)
https://goldbook.iupac.org/



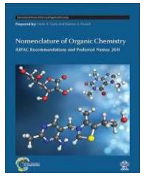
Green Book Quantities, Units and Symbols in Physical Chemistry
https://iupac.org/wp-content/uploads/2015/07/Green-Book-PDF-Version-2011.pdf



Red Book Nomenclature of Inorganic Chemistry
https://iupac.org/wp-content/uploads/2016/07/Red_Book_2005.pdf

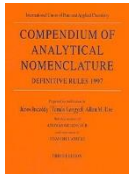


Blue Book Nomenclature of Organic Chemistry
https://www.acdlabs.com/iupac/nomenclature/



Purple Book Compendium of Polymer Terminology and Nomenclature
https://iupac.org/wp-content/uploads/2016/07/ONLINE-IUPAC-PB2-Online-June2014.pdf

Orange Book Analytical Chemistry
https://media.iupac.org/publications/analytical_compendium/



Principles of Chemical Nomenclature: A Guide to IUPAC Recommendations
https://iupac.org/wp-content/uploads/2018/05/principles_of_nomenclature98.pdf

Silver Book Compendium of Terminology and Nomenclature of Properties Clinical Laboratory Sciences

White Book Biochemical Nomenclature

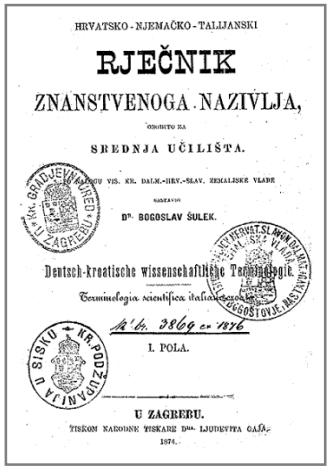
Hrvatska nomenklatura i terminologija kemije (1952 – 2019.)

1952. Godišnja skupština Hrvatskog kemijskog društva (**HKD**)
Odbor za kemijsku terminologiju i nomenklaturu

1964. Savez kemičara i tehnologa Hrvatske (današnje Hrvatsko društvo kemičara i kemijskih inženjera, **HDKI**)
Komisija za nomenklaturu i terminologiju organske kemije
70-tih godina započinje se s radom na hrvatskim prijevodima IUPAC-ovih preporuka

1974. Utemeljuje se **Komisija za terminologiju, jedinice i simbole HKD-a**
- sekcije za pojedina područja kemije;
- **Sekcija za nomenklaturu i terminologiju organske kemije**

1995. HKD i HDKI zajednička **Komisija za terminologiju i nomenklaturu**
- sekcije za pojedina područja kemije
Sekcija za nomenklaturu i terminologiju organske kemije
(Podsekcija za makromolekulsku kemiju)


HRVATSKO-NJEMAČKO-TALIJANSKI
RJEČNIK
ZNANSTVENOGA NAZIVLJA,
OSOBITO ZA
SREDNJA UČILIŠTA.
SASTAVIO
Dr. BOGOSLAV ŠULEK.
Deutsch-kroatische wissenschaftliche Terminologie.
Terminologia scientifica italiano-croata.
I. POLA.
U ZAGREBU.
1874.

Bogoslav Šulek
Hrvatsko-njemačko-talijanski rječnik znanstvenog nazivlja: osobito za srednja učilišta
Zagreb, 1874/1875.

IUPAC-ova pravila i preporuke za imenovanje (nomenklaturu) i grafičko prikazivanje aminokiselina i peptida

(preporuke HKD-a i HDKI-ja)

IUPAC-ova pravila i preporuke za nomenklaturu α-aminokiselina

Imena (trivijalna) uobičajenih α-aminokiselina	Troslovčani simboli	Jednoslovčani simboli
alanin	Ala	A
arginin	Arg	R
asparagin	Asn	N
asparaginska kiselina	Asp	D
cistein	Cys	C
fenilalanin	Phe	F
glicin	Gly	G
glutamin	Gln	Q
glutaminska kiselina	Glu	E
histidin	Hys	H
isoleucin	Ile	I
leucin	Leu	L
lizin	Lys	K
metionin	Met	M
prolin	Pro	P
serin	Ser	S
tirozin	Tyr	Y
treonin	Thr	T
triptofan	Trp	W
valin	Val	V
neodređena aminokiselina	Xaa	X

PHE = Pro-Hys-Glu

GLN = Gly-Leu-Asn

IUPAC-ova pravila i preporuke za nomenklaturu α-aminokiselina

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glutaminska kiselina	Glu	E
histidin	Hys	H
isoleucin	Ile	I
leucin	Leu	L
lizin	Lys	K
metionin	Met	M
prolin	Pro	P
serin	Ser	S
tirozin	Tyr	Y
treonin	Thr	T
triptofan	Trp	W
valin	Val	V
neodređena aminokiselina	Xaa	X

Asn, Asp → Asx; N, D → B

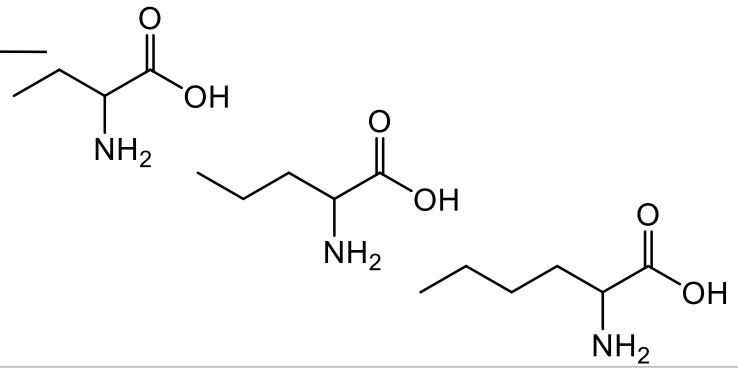
Gln, Glu → Glx ⇨ Gla, Glp; Q, E → Z

IUPAC-ova pravila i preporuke za nomenklaturu α-aminokiselina

Imena (trivijalna) rjeđih α-aminokiselina	Troslovčani simboli
β-alanin	βAla
aloizoleucin	aIle
alotreonin	aThr
allizin	–
citrulin	Cit
cistationin	Ala | Hcy
cisteinska kiselina	Cya
cistin	Cys | Cys

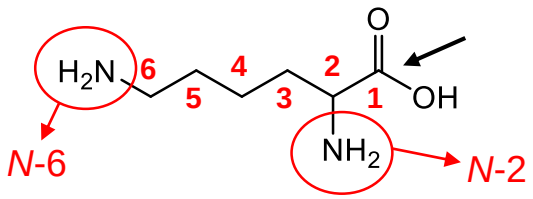
Imena (trivijalna) rjeđih α-aminokiselina	Troslovčani simboli
dopa	–
homocistein	Hcy
homoserin	Hse
homoserin lakton	Hsl
lantionin	Ala | Cys
ornitin	Orn
5-oksoprolin	Glp
sarkozin	Sar
tiroksin	Thx

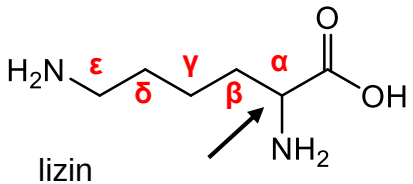
Trivijalna imena rjeđih α-aminokiselina	Supstitucijsko ime	Troslovčani simboli
homoalanin (AABA)	2-aminobutanska kiselina	Abu
norvalin (Nva)	2-aminopentanska kiselina	Ape
norleucin (Nle)	2-aminoheksanska kiselina	Ahx



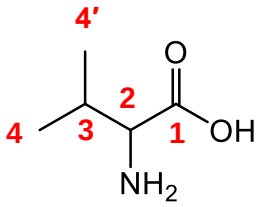
Numeriranje(obrojčavanje) α-aminokiselina

Acikličke aminokiseline

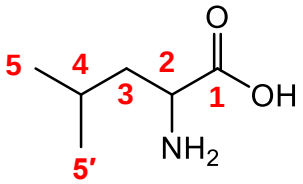




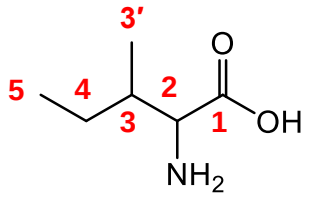
lizin



valin

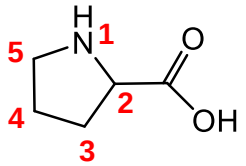


leucin



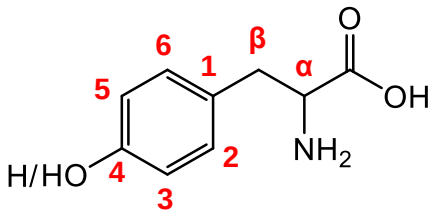
izoleucin

Cikličke aminokiseline

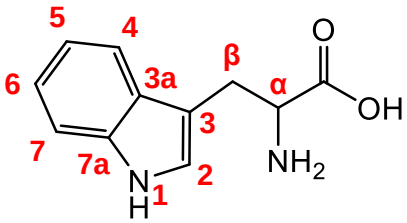


prolin

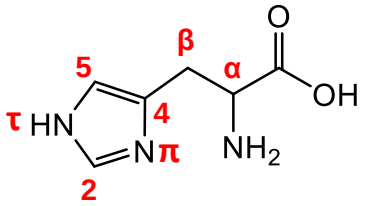
Aromatske aminokiseline



fenilalanin / tirozin



triptofan



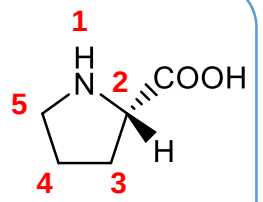
histidin

Deskriptori za označivanje konfiguracije α-aminokiselina

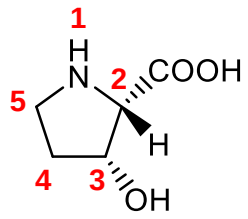
- Stereodeskriptori za α-ugljikov atom

  Apsolutna konfiguracija α-ugljikova atoma: **D** ili **L**

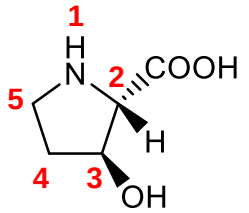
  Racemična smjesa: **DL** > *rac*



L-prolin (PIN)
(2S)-prolin



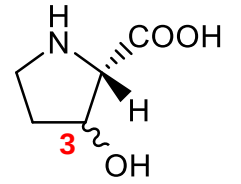
(3*R*)-3-hidroksi-L-prolin (PIN)
(2*S*,3*R*)-3-hidroksiprolin
cis-3-hidroksi-L-prolin

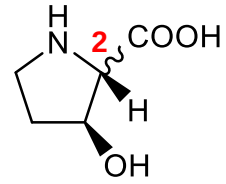


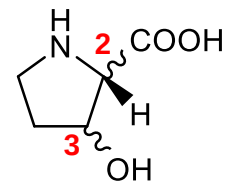
(3*S*)-3-hidroksi-L-prolin (PIN)
(2*S*,3*S*)-3-hidroksiprolin
trans-3-hidroksi-L-prolin

- Stereodeskriptori za kiralne ugljikove atome različite od α-ugljikova atoma ***R*** ili ***S*** (***R**** i ***S****)
- Preporuka zadržavanja specifičnih stereodeskriptora **D** ili **L** za označivanje α-ugljikova atoma i ***R*** ili ***S*** za ostale kiralne C-atome
- Stereodeskriptor za nepoznatu konfiguraciju C-atoma je **ζ**
- Deskriptori optičkog skretanja su **(+), (–),** racemična smjesa **(±)**

(+)-glutaminska kiselina
(+)-L-glutaminska kiselina
(±)-glutaminska kiselina

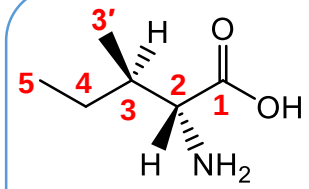




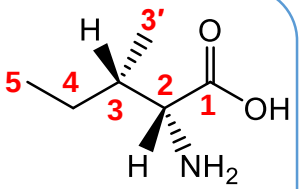


(2*S*,3*ζ*)-3-hidroksiprolin
(2*ζ*,3*ζ*)-3-hidroksiprolin
(2*ζ*,3*S*)-3-hidroksiprolin

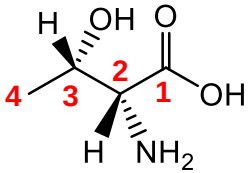
- Deskriptor ***mezo***
- Deskriptor **alo**



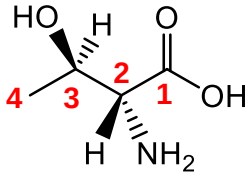
L-izoleucin
(simboli: Ile, I)



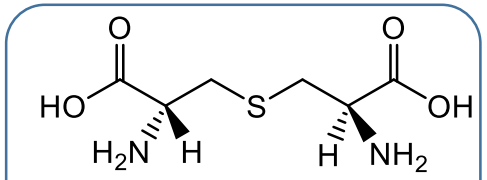
L-aloizoleucin
(simbol: aIle)



L-treonin
(simboli: Thr, T)



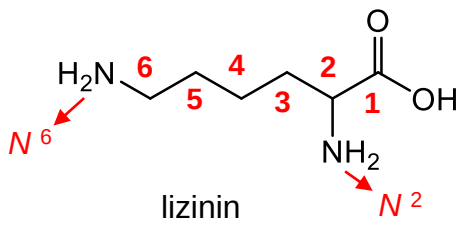
L-alotreonin
(simbol: aThr)

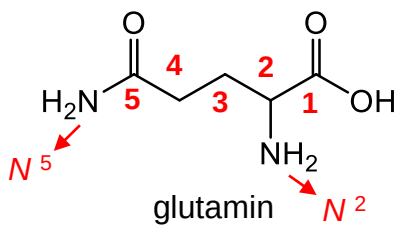


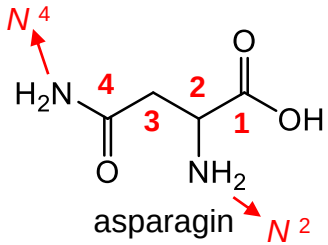
mezo-lantionin

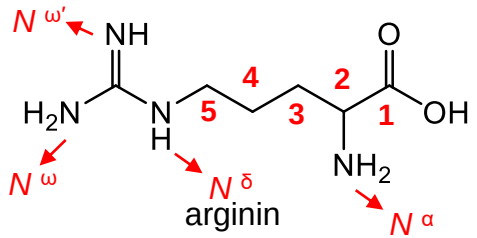
Nomenklatura (imenovanje) derivata α-aminokiselina

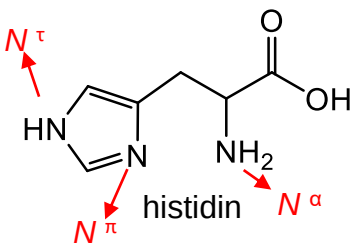
Označivanje lokanata α–aminokiselina s više od jedne amino-skupine



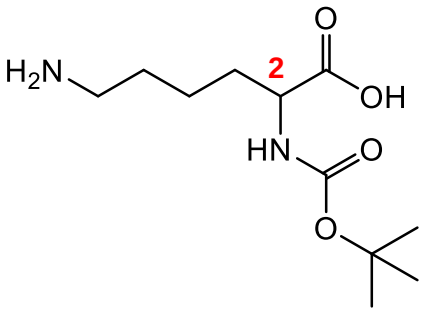




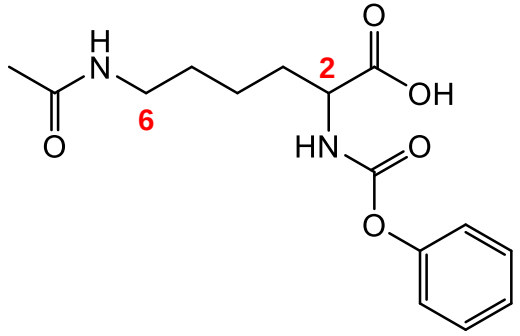




Supstitucija na amino-skupinama



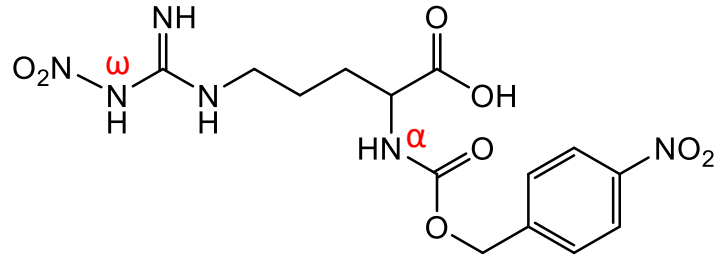
N 2-(*tert*-butiksikarbonil)-L-lizin



N 6-acetil-*N*2[(benziloksi)karbonil]-L-lizin

⇓

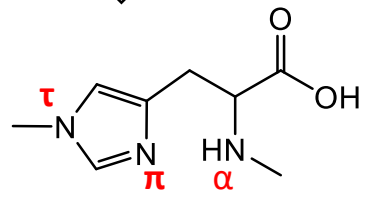
N 6-acetil-*N*2((benziloksi)karbonil)-L-lizin



N α-{[(4-nitrobenzil)oksi]karbonil]}-*N* ω-nitro-L-arginin

⇓

N α-(((4-nitrobenzil)oksi)karbonil))-*N* ω-nitro-L-arginin



N α,*N*τ-dimetil-L-arginin

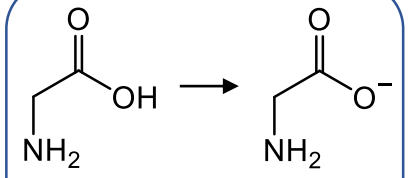
Zagrade:
( ) okrugle
[ ] uglate
{ } vitičaste

{ [({ [( )] })] }

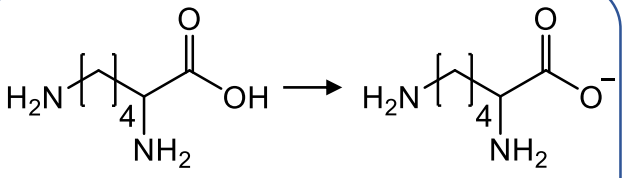
(3*S*)-2((2*S*)-2-{((1*S*)..... ⇨ (3*S*)-2[(2*S*)-2-{[(1*S*).....

Nomenklatura (imenovanje) ionizacijskih stanja α-aminokiselina

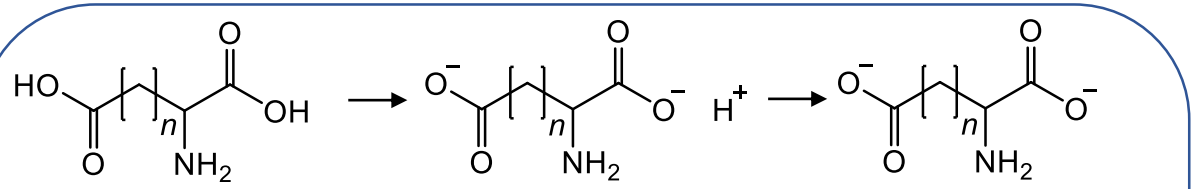
Ionizacija karboksilne skupine



glicin — glicinat, glicin-anion



leucin — leucinat, leucin-anion



***n*=1** asparaginska kiselina

aspartat(1–)
hidrogen-aspartat
asparaginska kiselina monoanion

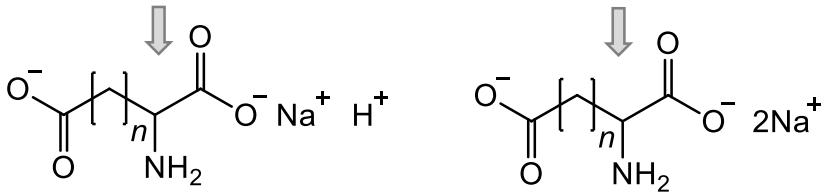
aspartat(2–)
asparaginska kiselina dianion = **aspartat**

***n*=2** glutaminska kiselina

glutamat(1–)
hidrogen-glutamat
glutaminska kiselina monoanion

glutamat(2–)
glutaminska kiselina dianion = **glutamat**

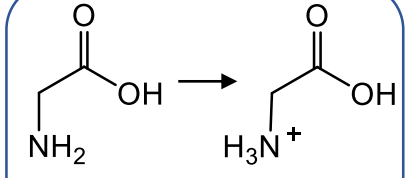
soli



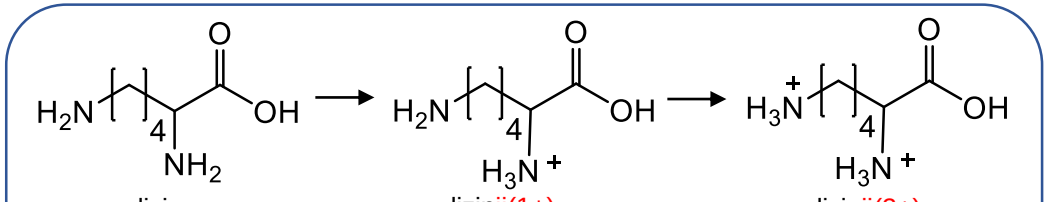
natrijev aspartat(1–) / glutamat(1–)
natrijev hidrogen-aspartat / hidrogen-glutamat

dinatrijev aspartat
dinatrijev glutamat

Ionizacija amino-skupine



glicin — glicinij, glicin-kation



lizin

lizinij(1+)
lizin-monokation
lizin-N^2-ij

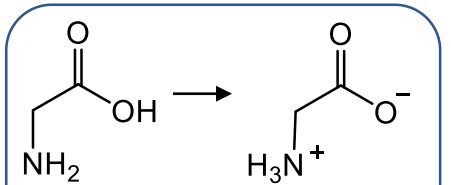
lizinij(2+)
lizin-dikation
lizin-N^2,N^6-ij

soli

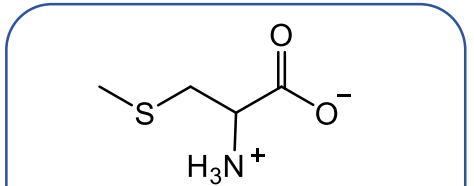
lizinij(1+) klorid

lizinij(2+) diklorid

Zwitterionski spojevi/zwitterioni (dipolni ioni)



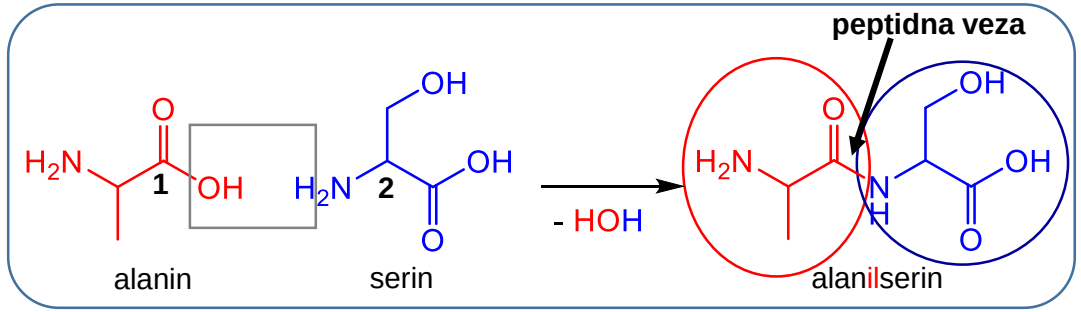
glicin — azanijilacetat, glicin-zwitterion



2-azanijil-3-(metilsulfanil)propanoat
S-metil-1-cistein-zwitterion

Nomenklatura (imenovanje) peptida

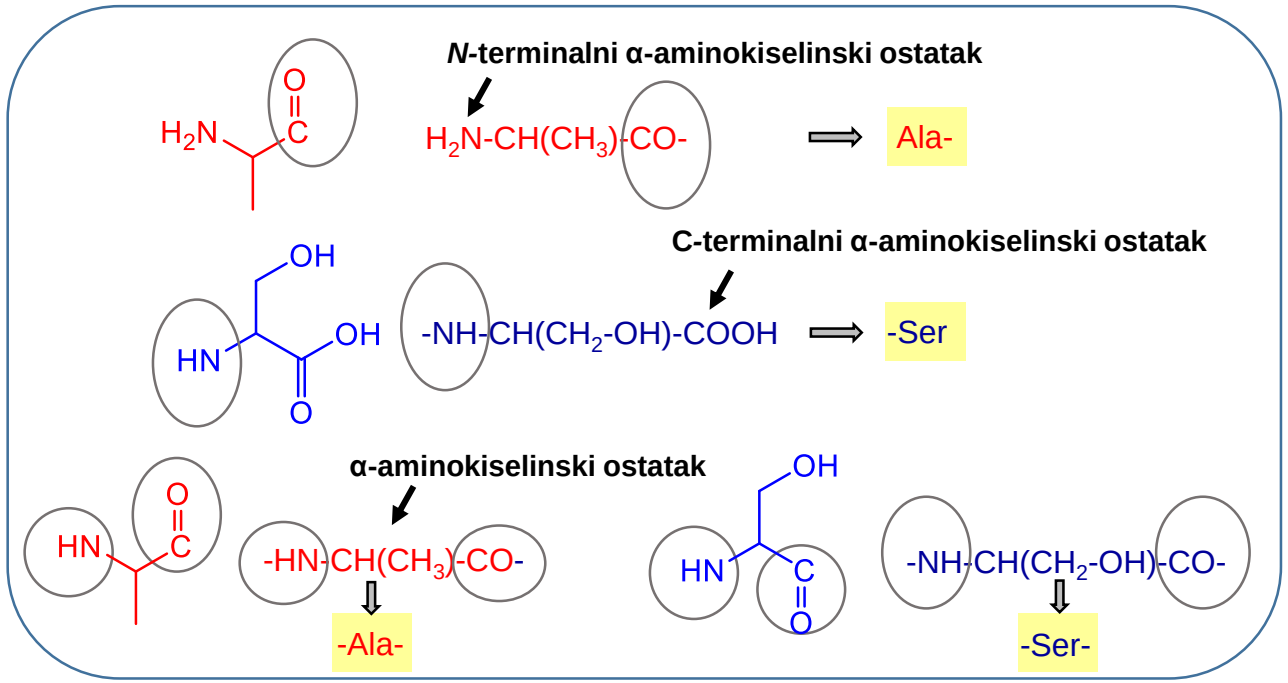
peptid / peptidna veza



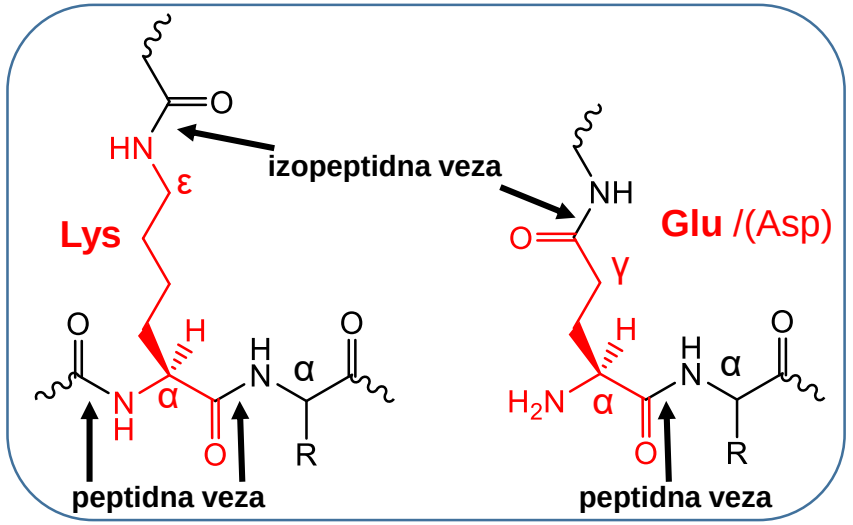
duljina peptidnog lanca

peptidi	**2 do 9 ak**	(di, tri, tetra.....)
oligopeptidi	**10 do 19 ak**	
polipeptidi	**20 do 49 ak**	
	(40 AK → tetrakontapeptid → **40-peptid**)	
	(Arg-Pro-Lys-Pro-Gln-Gln-Phe-Phe-Gly-Leu-Met → **supstanca P**)	
proteini	**> 50 ak ?**	

α-aminokiselinski ostatci



peptid / izopeptid



Nomenklatura (imenovanje) peptida

označivanje konfiguracije u peptidima

- α-aminokiseline **L**, **D**, **DL**, **ζ**
- peptidi **L**, **D**
  ambo (*rac*)
  ent
  ζ

L-leucil-D-glutamil-L-treonil-D-valil-L-leucin

leucil-D-glutamiltreonil-D-valilleucin

L-Leu-D-Glu-L-Thr-D-Val-L-Leu

Leu-D-Glu-Thr-D-Val-Leu

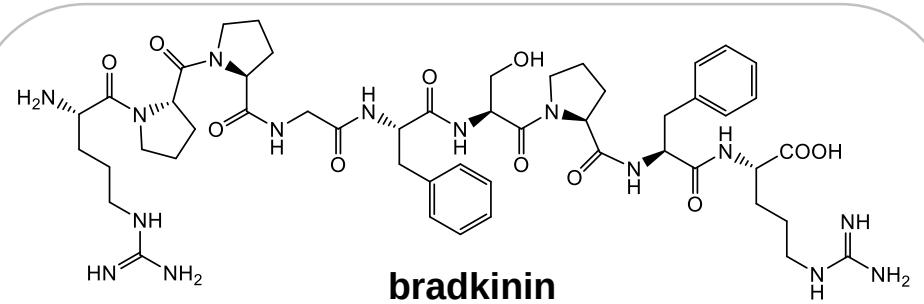
DL-alanil-DL-leucin

L-alanil-L-leucin
D-alanil-D-leucin
⟹ *rac*-L-alanil-L-leucin

L-alanil-D-leucin
D-alanil-L-leucin
⟹ *rac*-L-alanil-D-leucin

⇩

***ambo*-alanil-*ambo*-leucin**
***ambo*-Ala-*ambo*-Leu**



bradkinin

(Arg-Pro-Pro-Gly-Phe-Ser-Pro-Phe-Arg)

L-alanil-L-alanil-L-alanin
L-alanil-D-alanil-L-alanin

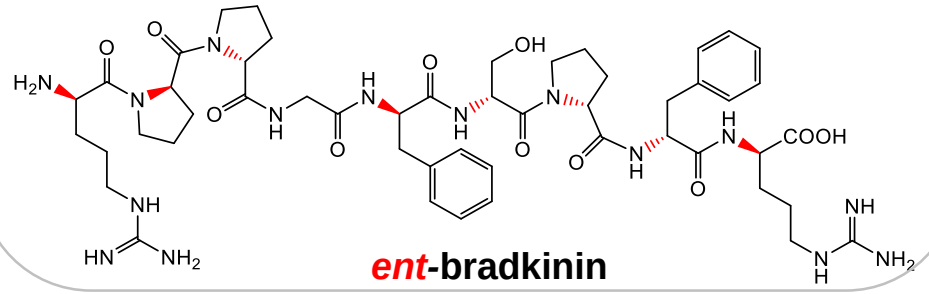
⇩

L-alanil-*ambo*-alanil-L-alanin

⇩

alanil-*ambo*-alanilalanin
Ala-*ambo*-Ala-Ala

alanil-*ζ*-alanilalanin
Ala-*ζ*-Ala-Ala



***ent*-bradkinin**

Nomenklatura (imenovanje) sintetski modificiranih prirodnih peptida

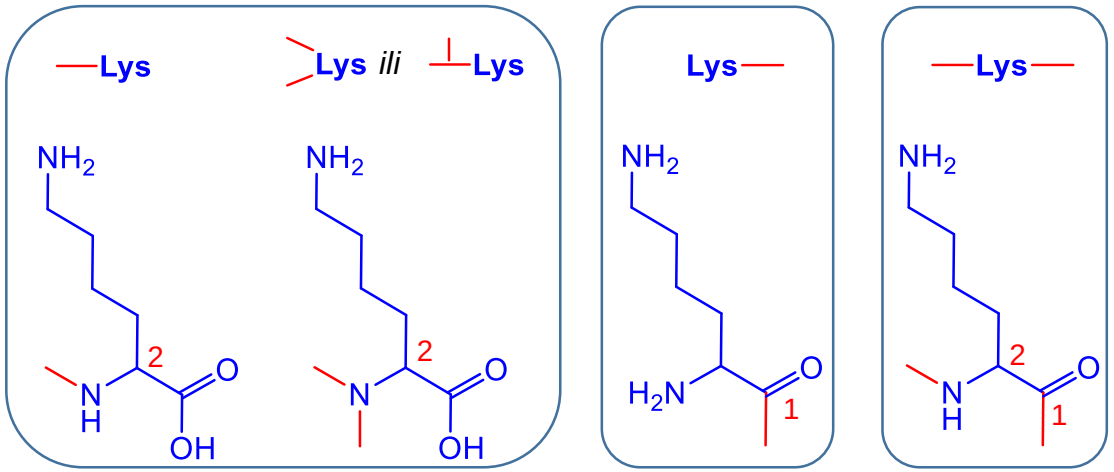
Operacija preinake	*Ime spoja*	*Formula*
	P E P T I D *(izmišljeni prirodni heksapeptid)*	**Phe-Glu-Phe-Thr-Ile-Asp** 1 2 3 4 5 6
▪ Zamjena jedne aminokiseline	[4-fenilalanin]P E P T I D [Phe^{4}]P E P T I D	**Phe-Glu-Phe-Phe-Ile-Asp** 4
dvije aminokiseline	[2-tirozin,4-fenilalanin]P E P T I D [Tyr^{2},Phe^{4}]P E P T I D	**Phe-Tyr-Phe-Phe-Ile-Asp** 2 4
▪ Produljenje na *N*-terminalnom kraju	fenilalanil-P E P T I D Phe-P E P T I D	**Phe-Phe-Glu-Phe-Thr-Ile-Asp** 1 6
▪ Produljenje na C-terminalnom kraju	P E P T I DIL-fenilalanin P E P T I DIL-Phe	**Phe-Glu-Phe-Thr-Ile-Asp-Phe** 1 6
▪ Umetanje jedne aminokiseline	endo-2a-fenilalanin-P E P T I D [endo-Phe^{2a}]-P E P T I D	**Phe-Glu-Phe-Phe-Thr-Ile-Asp** 1 2 2a 3 4 5 6
dvije aminokiseline	endo-2a-fenilalanin,3a-leucin-P E P T I D [endo-Phe^{2a},Leu^{3a}]-P E P T I D	**Phe-Glu-Phe-Thr-Leu-Phe-Ile-Asp** 1 2 2a 3 3a 4 5 6
▪ Uklanjanje aminokiseline	des-4-treonin-P E P T I D des-Thr^{4}-P E P T I D	**Phe-Glu-Phe-Ile-Asp** 1 2 3 5 6
▪ Supstitucija na karboksilnoj skupini bočnog lanca (glutaminske kiseline)	C$^{\gamma 2}$-P E P T I DIL-alanin C$^{\gamma 2}$-P E P T I DIL-Ala	Ala I γ **Phe-Glu-Phe-Thr-Ile-Asp** 1 2 3 4 5 6
▪ Fragment	P E P T I D-(2 – 4)tripeptid	**Glu-Phe-Thr** 2 3 4

Simboli α-aminokiselinskih ostataka

Monokarboksilne α-aminokiseline

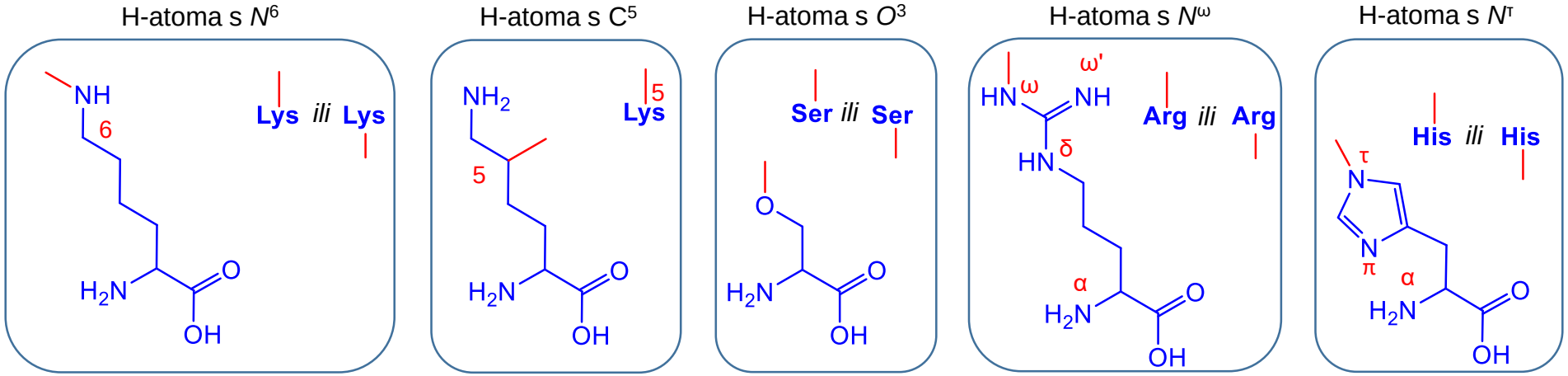
- **Uklanjanje H-atoma i/ili OH-skupine s „glavnog" lanca α-aminokiseline**

H-atom/atomi s N^2 | OH-skupine s C^1 | H-atom s N^2 i OH-skupina s C^1



- **Uklanjanje H-atoma s bočnog lanca α-aminokiseline**

H-atoma s N^6 | H-atoma s C^5 | H-atoma s O^3 | H-atoma s N^{ω} | H-atoma s N^{τ}



Simboli α-aminokiselinskih ostataka

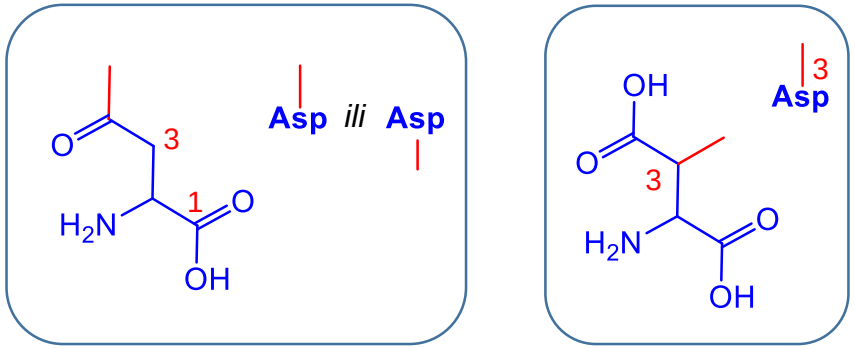
Dikarboksilne α-aminokiseline

- **Uklanjanje H-atoma i/ili OH-skupine s „glavnog" lanca α-aminokiseline**

H-atom/atomi s N^2 | OH-skupine s C^1 | H-atom s N^2 i OH-skupina s C^1

- **Uklanjanje H-atoma ili OH-skupine s bočnog lanca α-aminokiseline**

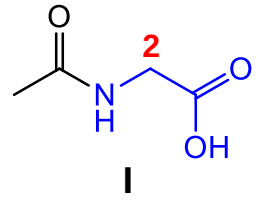
OH-skupine s COOH na C^3 | H-atoma s C^3



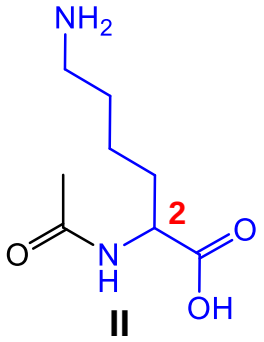
Primjeri simbola supstituiranih α-aminokiselina

Supstitucija na *N*-terminalnom kraju (2-amino-skupina)

N-acetilglicin Ac-Gly **I**
N^2-acetillizin Ac-Lys **II**



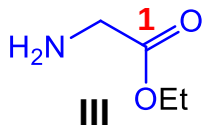
I



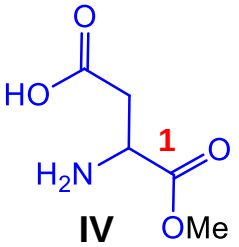
II

Supstitucija na C-terminalnom kraju (1-karboksilna skupina)

glicin-etil-ester Gly-OEt **III**
O^1-metil-hidrogen-aspartat Asp-OMe **IV**



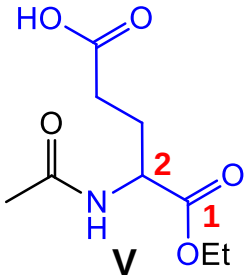
III



IV

Supstitucija na *N*- i C-terminalnim krajevima

O^1-etil-*N*-acetilglutamat Ac-Glu-OEt **V**

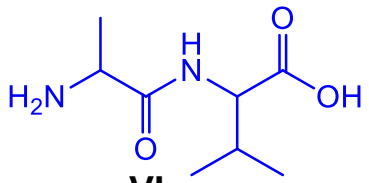


V

Primjeri simbola supstituiranih α-aminokiselina

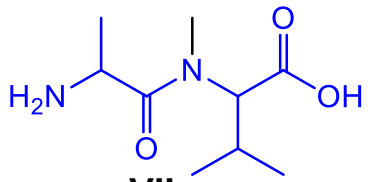
mono- i disupstituirane amino-skupine u peptidima na primjeru dipeptida

alanilvalin Ala–Val **VI**



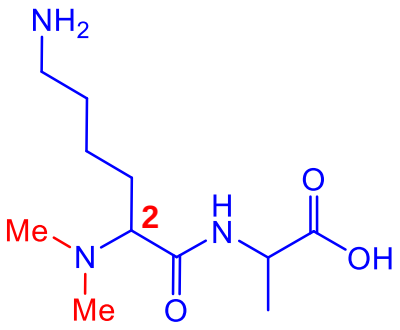
VI

alanil-*N*-metilvalin Ala–Val *ili* Ala-(Me)Val **VII**

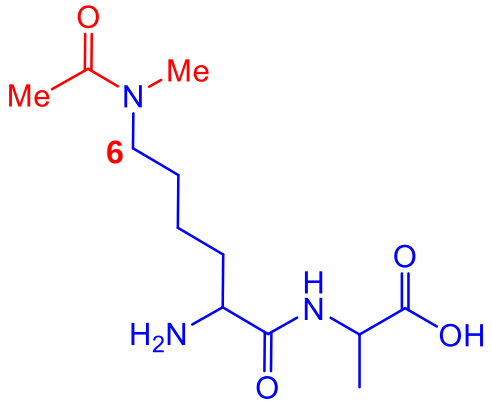


VII

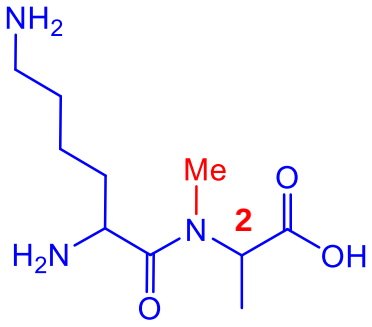
Me_2-Lys-Ala	disupstituirana N^2-amino-skupina lizina u lizilalaninu	**VIII**
Lys(Ac,Me)-Ala	disupstituirana N^6-amino-skupina lizina u lizilalaninu	**IX**
Lys-(Me)Ala	monosupstituirana N^2-amino-skupina alanina u lizilalaninu	**X**
Lys(Me)-Ala	monosupstituirana N^6-amino-skupina lizina u lizilalaninu	**XI**



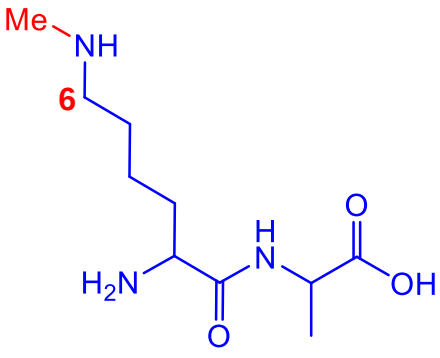
VIII



IX



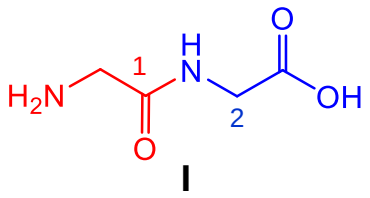
X



XI

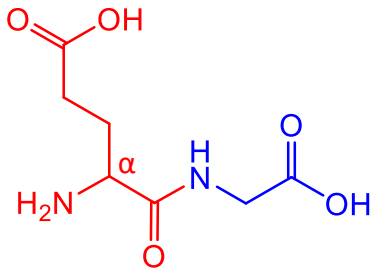
Primjeri simbola peptida s peptidnom vezom na bočnom lancu α-aminokiselina

glicilglicin Gly–Gly **I**



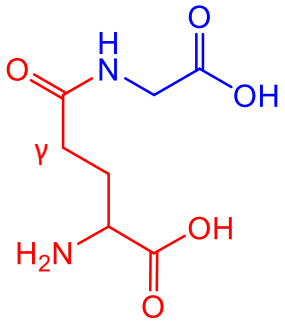
I

N-α-glutamilglicin Glu–Gly **II**



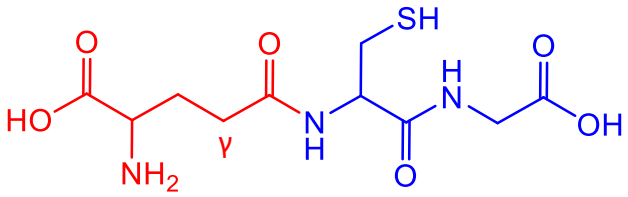
II

N-γ-glutamilglicin Glu —Gly *ili* Glu(—Gly) **III**

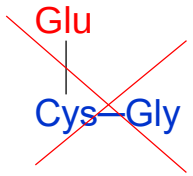


III

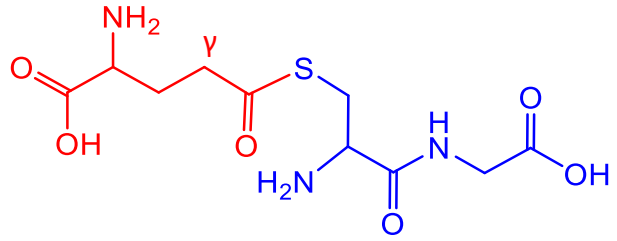
N-γ-glutamilcisteinilglicin (glutation) Glu —Cys—Gly *ili* Glu(—Cys—Gly) **IV**



IV



IV

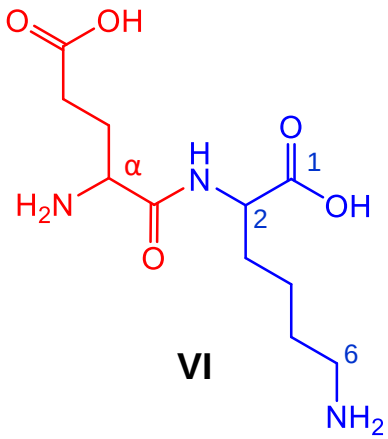


Primjeri simbola peptida s peptidnom vezom na bočnom lancu α-aminokiselina

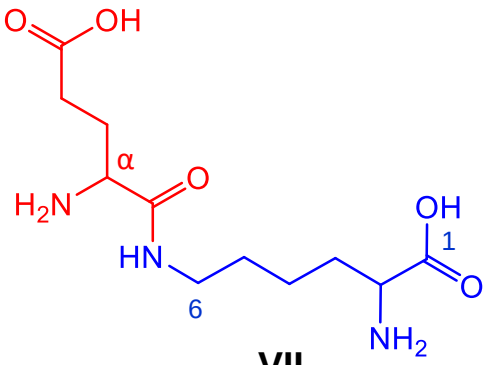
obje aminokiseline imaju funkcijsku skupinu na bočnom lancu

N^2-α-glutamillizin Glu–Lys **VI**

N^6-α-glutamillizin Glu(–Lys) *ili* Glu(–Lys) **VII**



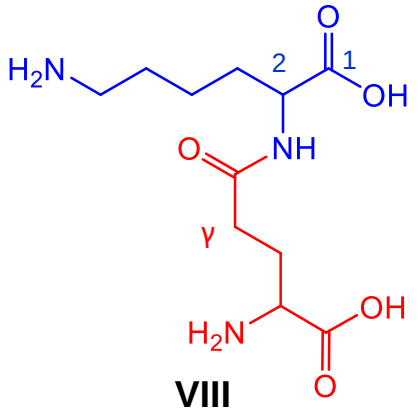
VI



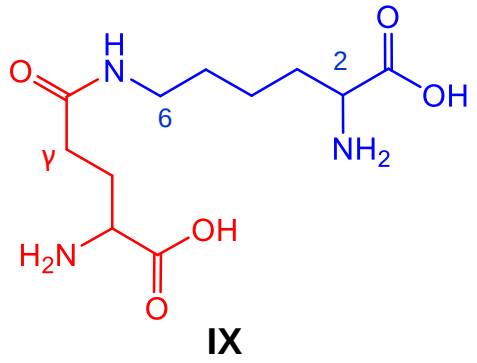
VII

N^2-γ-glutamillizin Glu(–Lys) *ili* Glu(–Lys) VIII

N^6-γ-glutamillizin Glu(–Lys) *ili* Glu Lys *ili* Glu Lys **IX**



VIII



IX

ZAHVALA

kolegicama i kolegama kemičarima koji su od samog začetka ideje o potrebi za nomenklaturom i terminologijom kemije na hrvatskom jeziku,
pa sve do danas,
kroz prijevode IUPAC-ovih preporuka,
doprinijeli da se hrvatski strukovni jezik kemije sačuva i dalje izgrađuje.