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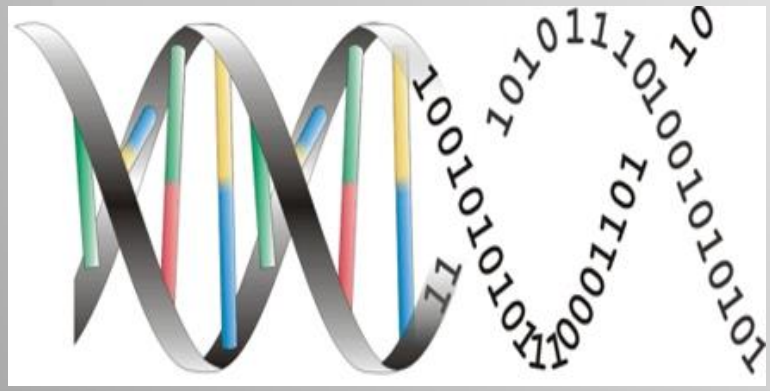
Programming for Computational & Systems Biology

Instructor: Paul Xie

Tue. & Thr. 9:35~10:50



Overview of Course

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- Introduction to programming skills in computational and systems biology. Topics include real world examples, such as processing genome or proteome data, and analyzing large-scale data. The idea of “big data” will be emphasized to help students with their coding skills to discovering new knowledge in biomedical sciences and solving biomedical problems.

Course Format

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- Computer labs + lectures (3 hours/week)
- Coding concepts (some knowledge about biological data)
- 6-8 assignments, published on eLC, (30-40%)
  - Please upload them by the due days
- Paper review (10-20%)
- 1 term paper (50-60%)

Topics

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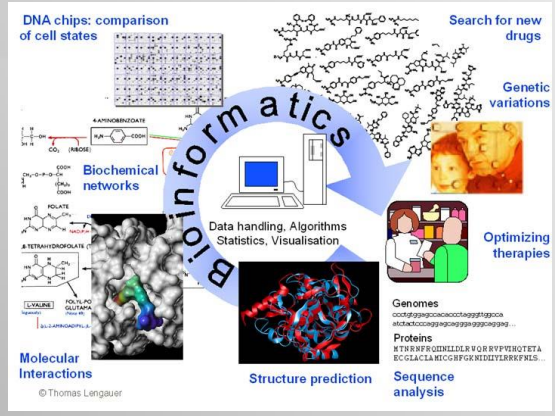
- -Omics data, e.g. Genomics, Proteomics…
- Basic Programming, e.g. I/O, variables, string, loop, regular express, array…etc.
- Data retrieval & processing
- Data analysis
- Model & building model
- Clustering and Classification
- Prediction



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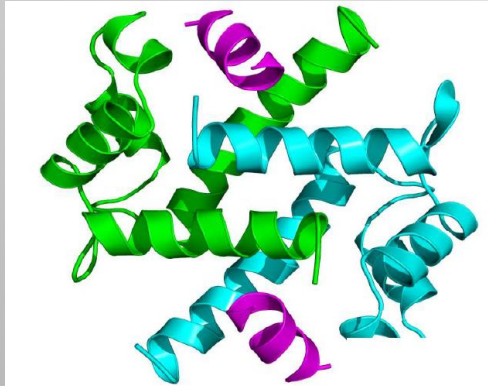
Regular Expression
Amino Acid & Protein Structure

Instructor: Paul Xie (7)



Last Week

- Sequence alignment
  - Global (N-W) and Local (S-W)
- Statistics model & Blast
- List
- Random number

This Week

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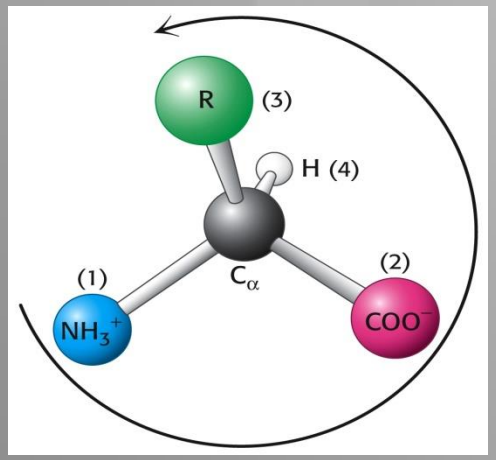
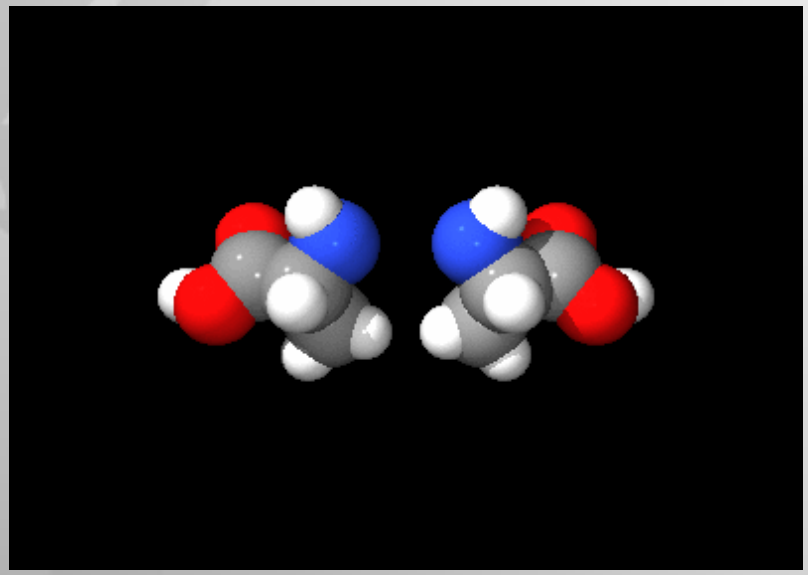
- Amino Acids & Protein
- Regular expression





Python Time

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Syntax

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- Regular expression
  - import re
  - re.search
    - Example:
    - print(x)
    - print(x.string)
    - Print(x.group())
  - re.match
  - re.findall
  - re.split
  - re.sub

Example

- S = ‘it rains in Spain’
  - re.search(pattern, string)

Syntax

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- Regular expression
  - metacharacters
  - . ^ $ * + ? { } [ ] \ | ( )
  - [] ➔ any character in the bracket, e.g. [A-Z]
  - () ➔ the specific pattern should be stored
  - | ➔ or e.g. A|T|C|G == [ATCG]
  - \ ➔ escape the original meaning e.g. \d == [0-9], \w == [a-zA-Z0-9], \s == any spaces, \n == new line

Example

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- fruit = ['1 @pple#$&', '3 oranges', '5 grapes', '7 peaches', '9 blue berries', '11 pineapples', '12 lemons']


TIME
FOR A
BREAK

Structures

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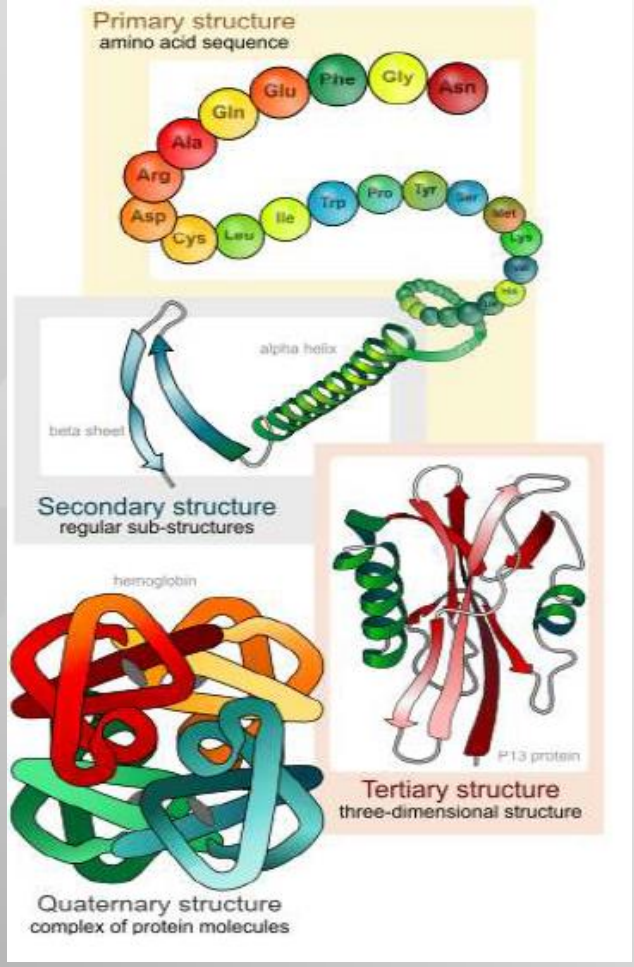
- Protein structures
  - Primary (sequence)
  - Secondary (helix, sheet, turn)
  - Motifs (Super-secondary)
  - Tertiary
  - Quaternary



Secondary Structures

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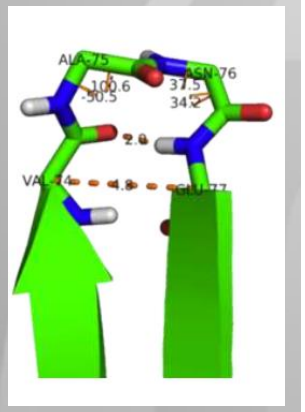
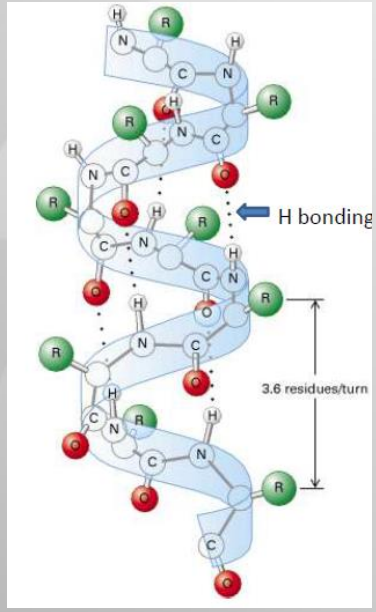
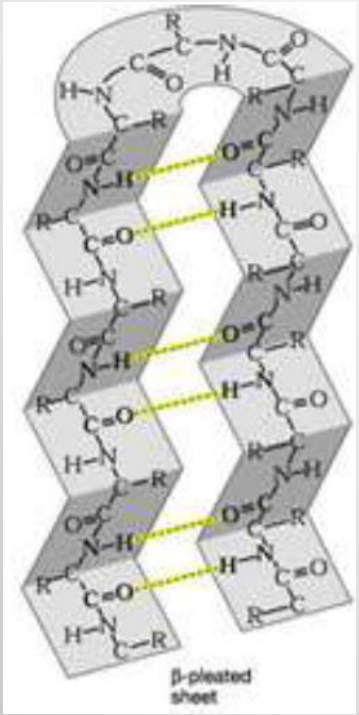
- Secondary structures
  - Alpha helix
  - Beta sheet
  - Tight turn
  - Loop

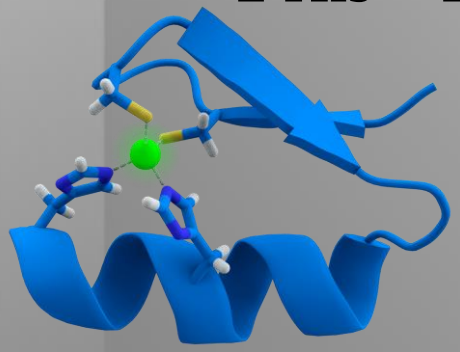


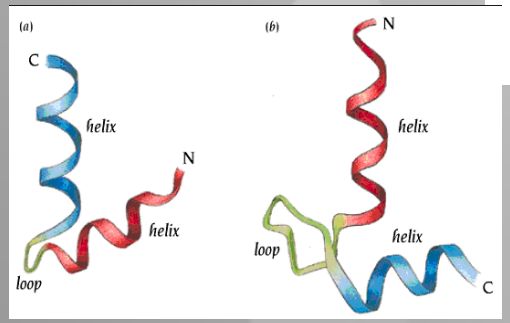


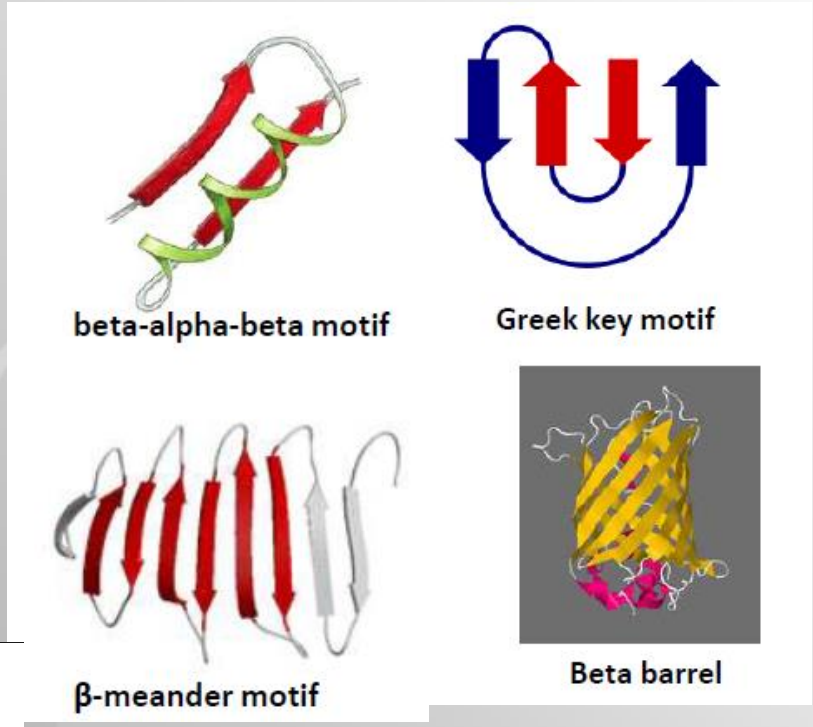


Motifs

- Beta-alpha-beta
- HLH
- Greek key
- Zinc finger
  - 2 His + 2 Cys + Zn

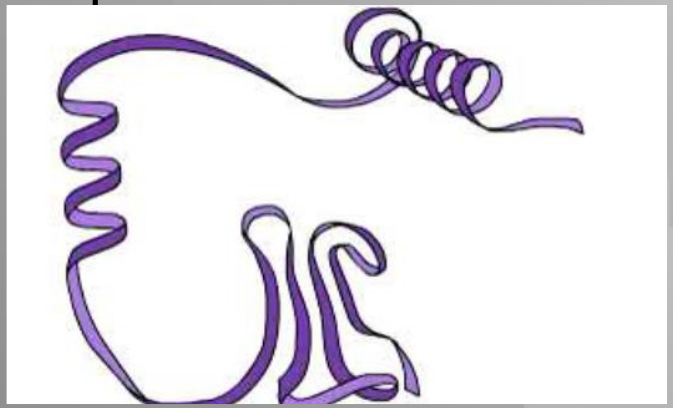


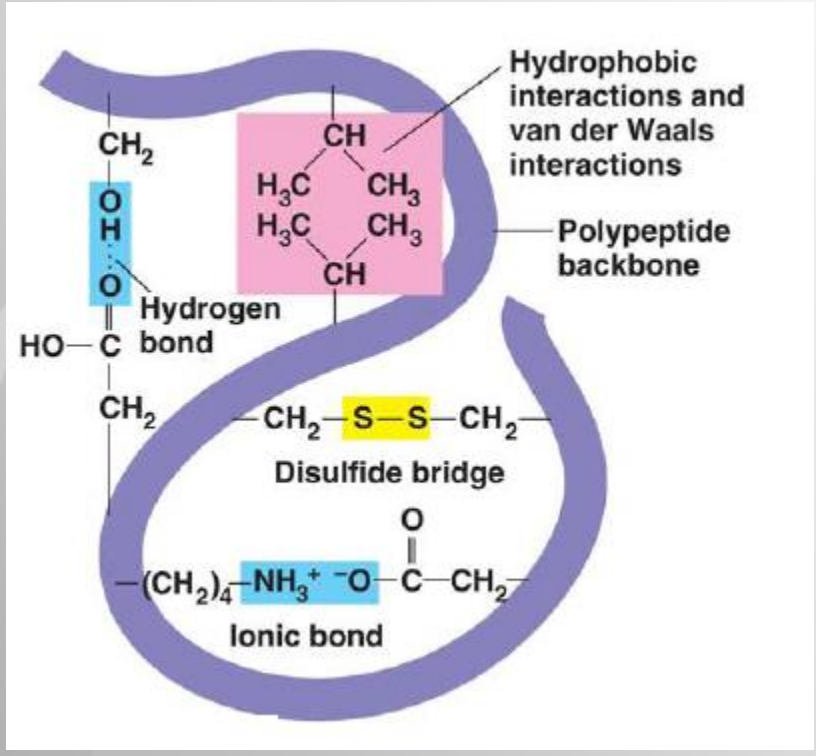




Interactions

- Interactions stabilize 3D structures
  - Hydrogen bond
  - Ionic bonds
  - Disulfide bonds
  - Hydrophobic interactions





Classification

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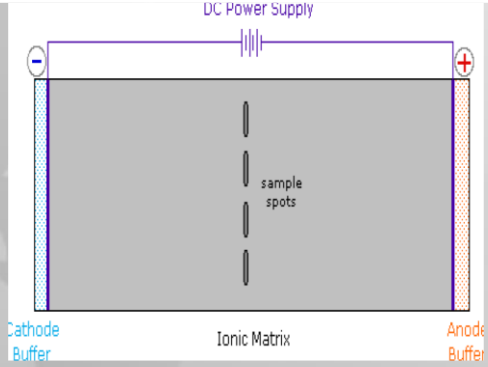
- Enzymes (Ligase)
- Transport proteins (Hemoglobin)
- Storage Proteins (Ferritin)
- Contractile/Motile Proteins (Actin)
- Regulatory Proteins (Hormones, insulin)
- Receptors (Estrogen receptor)

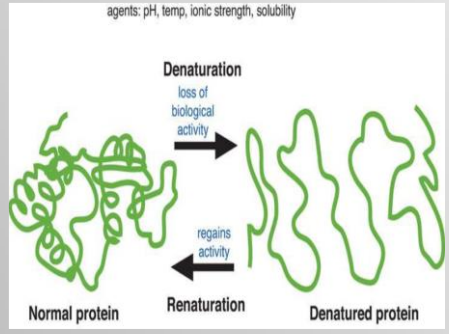
Property

- Henderson-Hasselbalch Equation

Henderson-Hasselbalch Equation: $pK_a = pH + \log \frac{[HA]}{[A^-]}$

- Isoelectric point (pI)
- Electrophoresis
- Folding & denature
  - Alcohol, salt, acid & base





Properties and Conventions Associated with the Standard Amino Acids

Amino acid	Abbreviated names		M_r	pK_a values: pK_1 (—COOH)	pK_2 ($—NH_3^+$)	pK_R (R group)	pI	Hydropathy index*	Occurrence in proteins (%)†
Nonpolar, aliphatic R groups									
Glycine	Gly	G	75	2.34	9.60		5.97	−0.4	7.2
Alanine	Ala	A	89	2.34	9.69		6.01	1.8	7.8
Valine	Val	V	117	2.32	9.62		5.97	4.2	6.6
Leucine	Leu	L	131	2.36	9.60		5.98	3.8	9.1
Isoleucine	Ile	I	131	2.36	9.68		6.02	4.5	5.3
Methionine	Met	M	149	2.28	9.21		5.74	1.9	2.3
Aromatic R groups									
Phenylalanine	Phe	F	165	1.83	9.13		5.48	2.8	3.9
Tyrosine	Tyr	Y	181	2.20	9.11	10.07	5.66	−1.3	3.2
Tryptophan	Trp	W	204	2.38	9.39		5.89	−0.9	1.4
Polar, uncharged R groups									
Serine	Ser	S	105	2.21	9.15		5.68	−0.8	6.8
Proline	Pro	P	115	1.99	10.96		6.48	1.6	5.2
Threonine	Thr	T	119	2.11	9.62		5.87	−0.7	5.9
Cysteine	Cys	C	121	1.96	10.28	8.18	5.07	2.5	1.9
Asparagine	Asn	N	132	2.02	8.80		5.41	−3.5	4.3
Glutamine	Gln	Q	146	2.17	9.13		5.65	−3.5	4.2
Positively charged R groups									
Lysine	Lys	K	146	2.18	8.95	10.53	9.74	−3.9	5.9
Histidine	His	H	155	1.82	9.17	6.00	7.59	−3.2	2.3
Arginine	Arg	R	174	2.17	9.04	12.48	10.76	−4.5	5.1
Negatively charged R groups									
Aspartate	Asp	D	133	1.88	9.60	3.65	2.77	−3.5	5.3
Glutamate	Glu	E	147	2.19	9.67	4.25	3.22	−3.5	6.3

Enzyme

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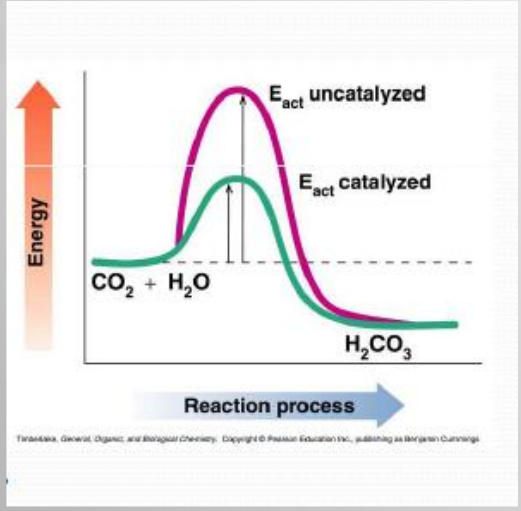
- In Greek means in living (en=in, zyme=living)
- Biocatalysts or Organic catalysts
- Increase the reaction rate
  - By lowering the energy of activation
- Catalyze the chemical reactions in the cell



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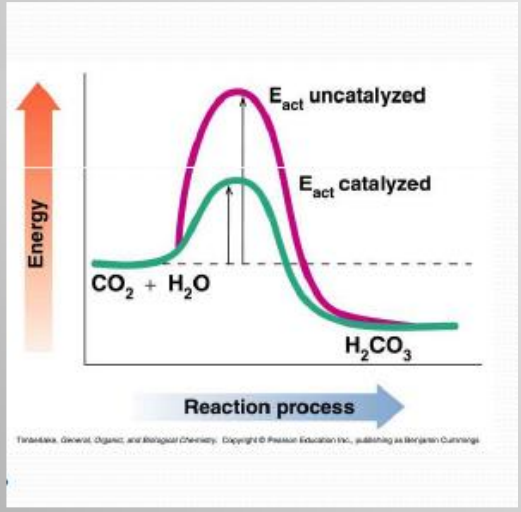

Nomination & Classification

- Usually ends in –ase (DNA Polymearse)
- Substrate & reaction catalyzed
  - Lactate dehydrogenase
- EC (Enzyme commission) no.
  - e.g. 1.1.1.1 alcohol dehydrogenase

EC Number

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- 6 groups

Top-level EC numbers[5]

Group	Reaction catalyzed	Typical reaction	Enzyme example(s) with trivial name
EC 1 ***Oxidoreductases***	To catalyze oxidation/reduction reactions; transfer of H and O atoms or electrons from one substance to another	AH + B → A + BH (**reduced**) A + O → AO (**oxidized**)	Dehydrogenase, oxidase
EC 2 ***Transferases***	Transfer of a functional group from one substance to another. The group may be methyl-, acyl-, amino- or phosphate group	AB + C → A + BC	Transaminase, kinase
EC 3 ***Hydrolases***	Formation of two products from a substrate by hydrolysis	AB + H_2O → AOH + BH	Lipase, amylase, peptidase
EC 4 ***Lyases***	Non-hydrolytic addition or removal of groups from substrates. C-C, C-N, C-O or C-S bonds may be cleaved	RCOCOOH → RCOH + CO_2or [X-A+B-Y] → [A=B + X-Y]	Decarboxylase
EC 5 ***Isomerases***	Intramolecule rearrangement, i.e. isomerization changes within a single molecule	ABC → BCA	Isomerase, mutase
EC 6 ***Ligases***	Join together two molecules by synthesis of new C-O, C-S, C-N or C-C bonds with simultaneous breakdown of ATP	X + Y+ ATP → XY + ADP + Pi	Synthetase

Catalysis

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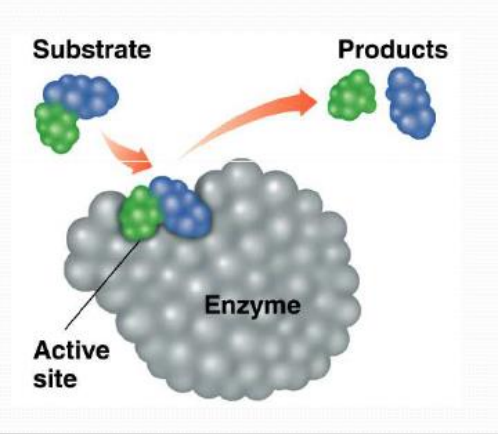
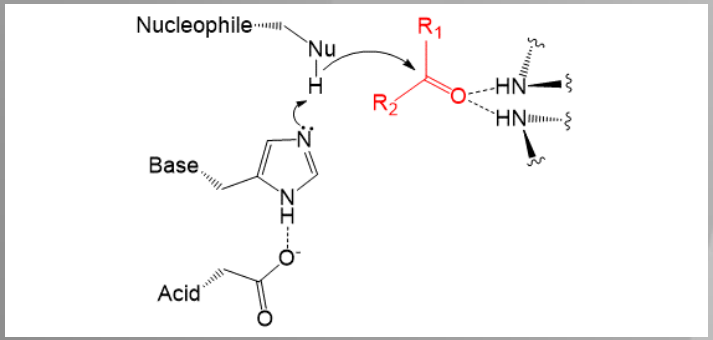
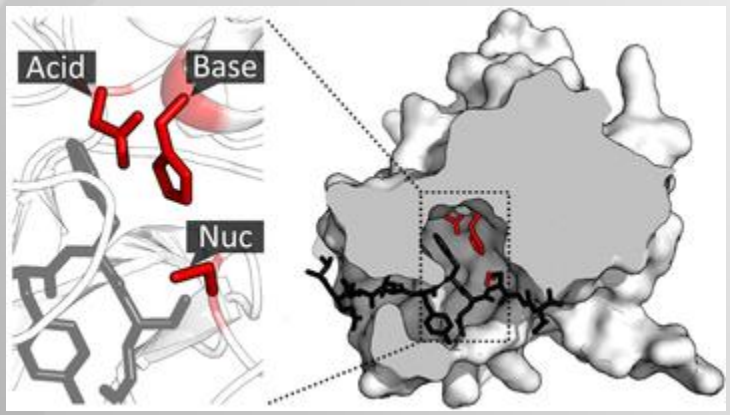
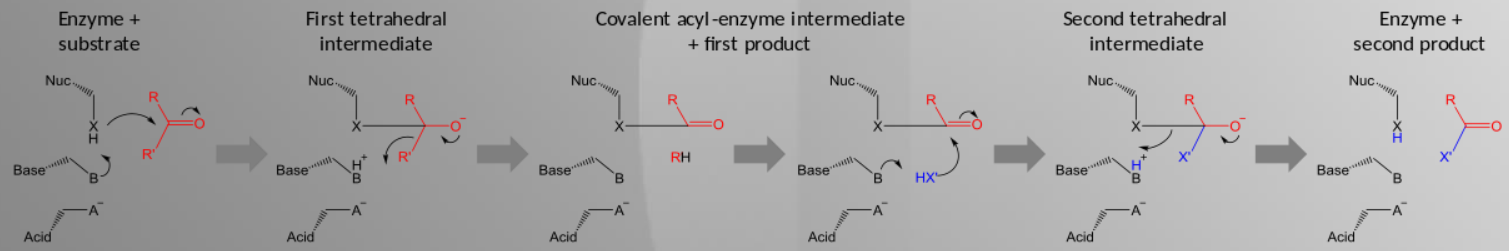
- Active sites
- Catalytic triad
  - Hydrolase or transferase
  - Acid, base, & nucleophile









Inhibition

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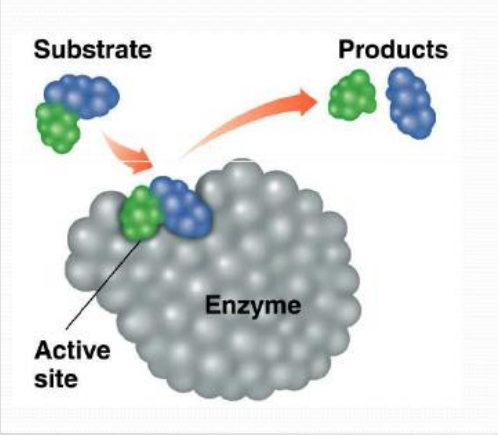
- Different ways to inhibit enzymes
  - Drug binding
    - Competitive inhibition
  - Conformational change
    - Uncompetitive inhibition
  - Covalent bonding
  - Denature
  - Change pH




TIME
FOR A
BREAK

This Week

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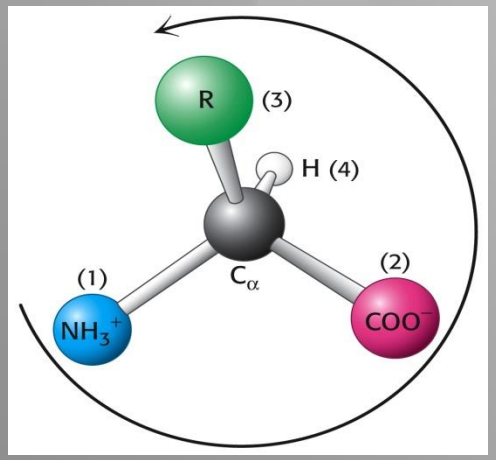
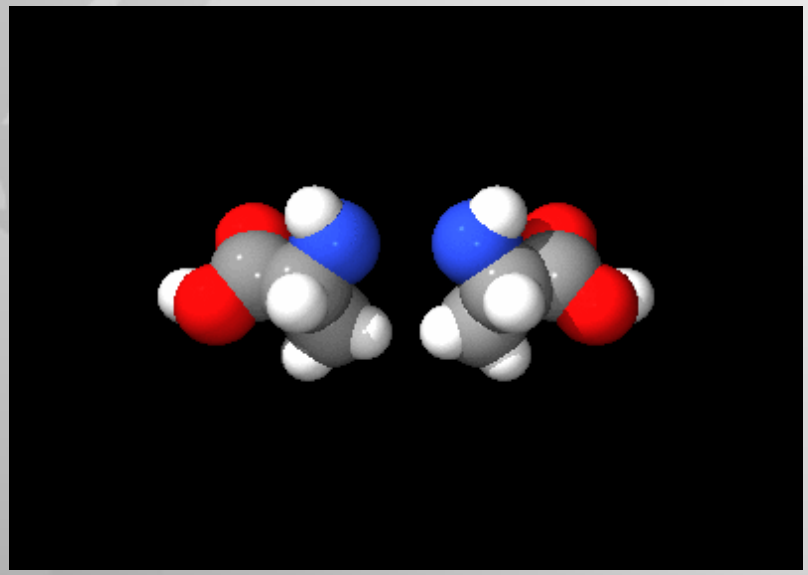
- Amino Acids
- Regular expression





Functions of amino acids

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- A variety of roles in metabolism
  - the building blocks of proteins
  - forming parts of coenzymes
  - as precursors for the biosynthesis of molecules such as heme

Standard and nonstandard amino acids

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- More than 300 different amino acids have been described in nature.
  - Standard α-amino acids:
    - Only *20 are commonly found as constituens of proteins*
  - Nonstandard amino acids:
    - Amino acid derivatives found in protein
    - Non-protein amino acid

- Why are amino acids uniquely suited to their role as the building blocks of proteins?

General structure of α-amino acids *(Very important!)*

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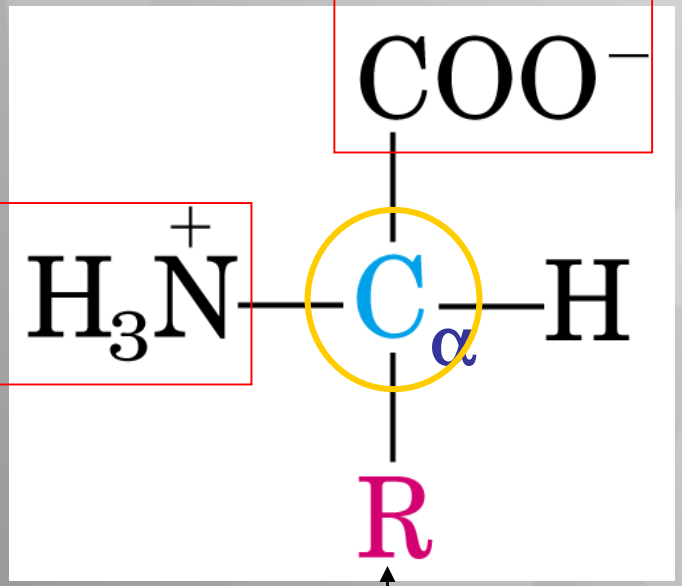
- carboxyl group

amino group

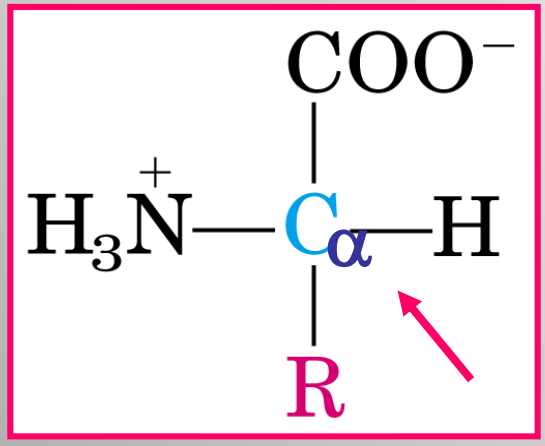


side chain

(or R group, R="Remainder of the molecule")

Stereochemistry of amino acids

- Configuration
- For all the common amino acids except Glycine, the α-carbon is bonded to four different groups.
- The α-carbon atom is thus a chiral center.

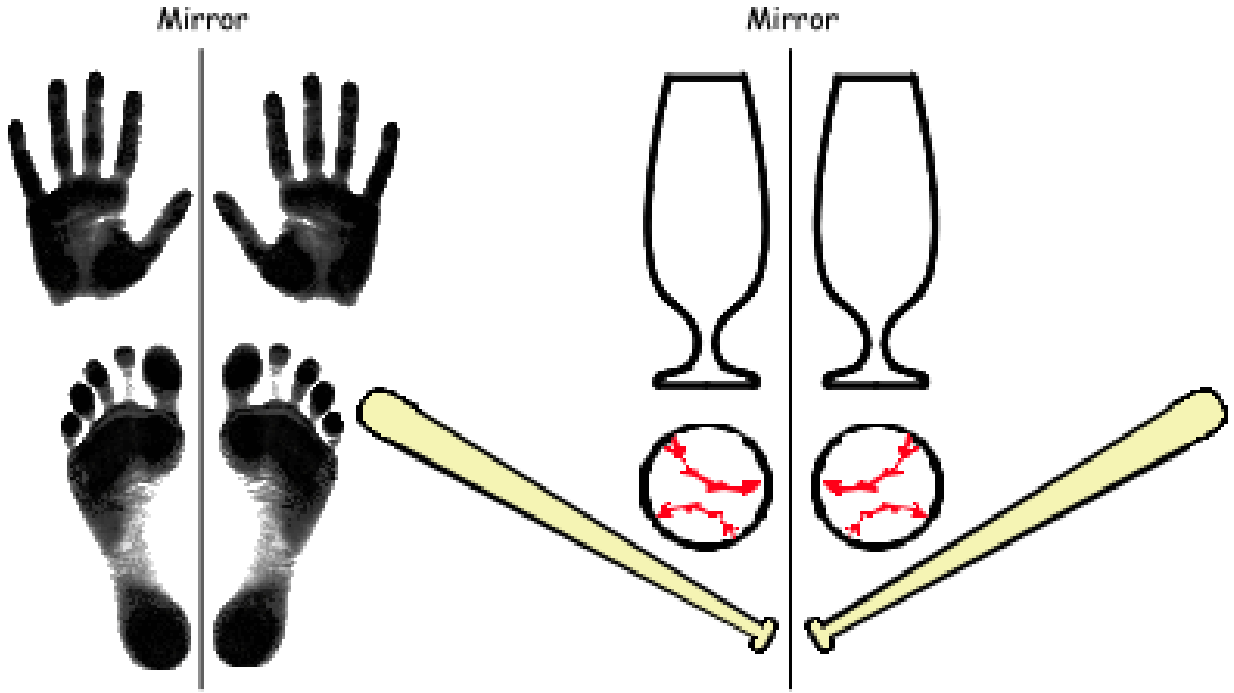


Chiral

- Chiral (from Greek *cheir*, meaning "hand"):
  - An object or a system cannot be superimposed on its mirror image.
  - One hand does not match the other when superimposed.

CHIRALITY

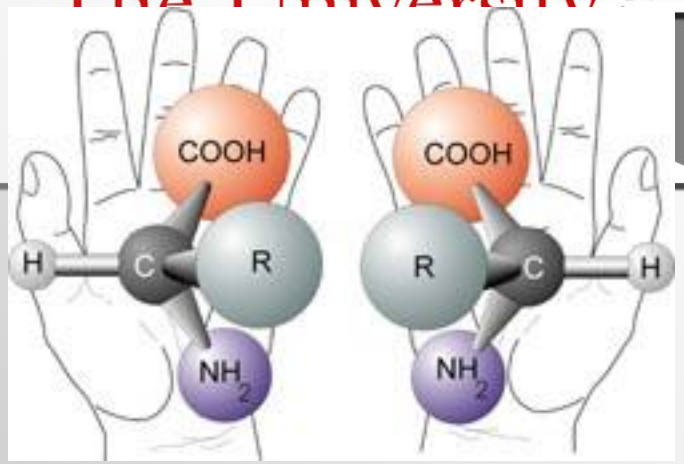
An object that cannot be superimposed on its mirror image is called chiral



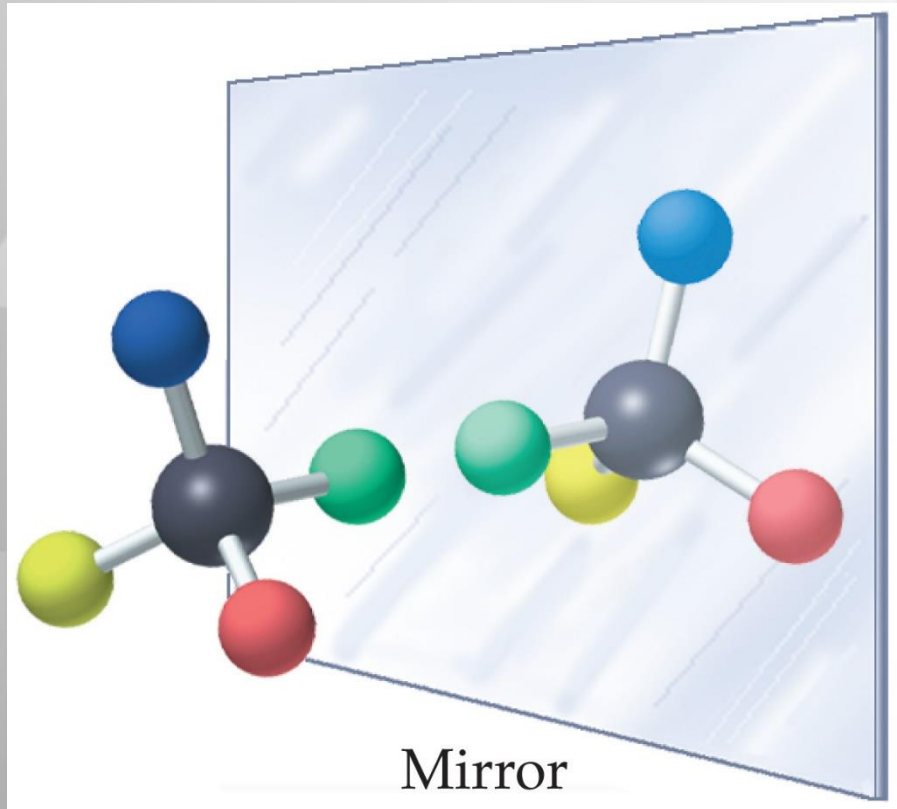
Chiral objects
Nonsuperimposable
mirror images

Nonchiral objects
Superimposable
mirror images

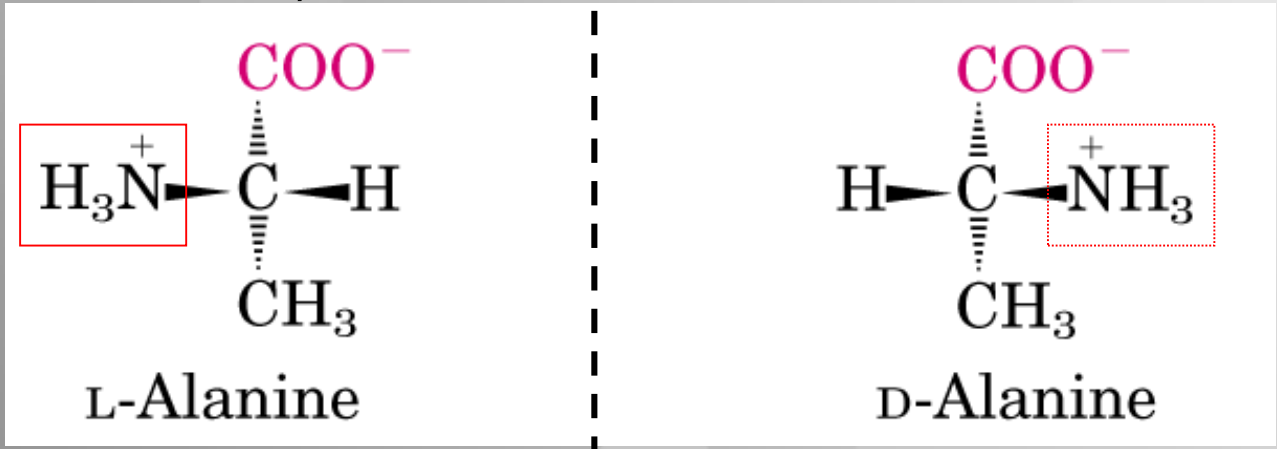
Chiral molecule



- Chiral molecule:
  - if a molecule has an atom bonded to four different groups, it can be chiral.



- The two enantiomers of each amino acid are designated by D,L system according to the D- and L-glyceraldehyde.
- D: Dextrorotation; L: Levorotation



- **Only the *L-amino acids* have been found in proteins.**
- (D-isomers have been found only in small peptides of bacteria cell walls or in some peptide antibiotics).

The Classification of 20 standard Amino Acids (*very important!!!*)

- The name and abbreviation of amino acids
  - All the AAs were given a trivial (common) name.
    - Glutamate from wheat gluten.
    - Tyrosine from cheese ("tyros" in Greek).
  - Each AA is given a 3 letter abbreviation and 1 letter symbol.
    - They often the first three letter and the first letter. When there is confusion, an alternative is used.
- They should be remembered !

Classification of Amino Acids

- Based on polarity
  - Nonpolar, aliphatic amino acids
  - Polar, uncharged amino acids
  - Acidic amino acids
  - Basic amino acids
  - Aromatic amino acids

Aliphatic Amino Acids:

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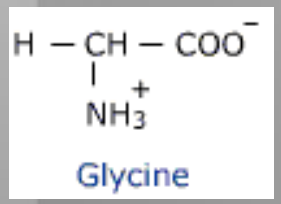
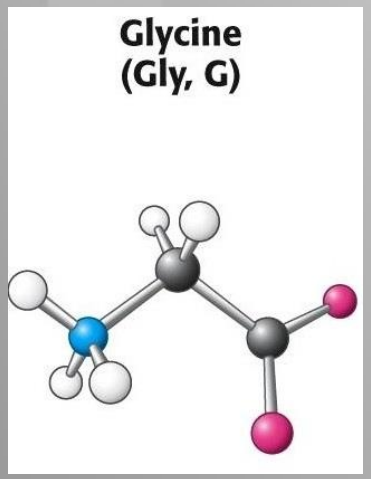
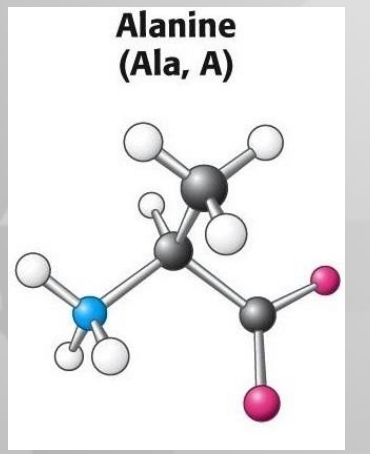
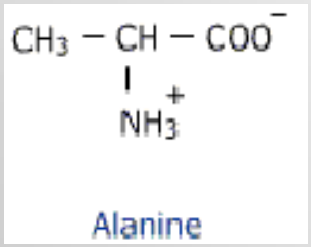
a) Mono-amino mono-carboxylic acids:

- Simple amino acids: Glycine , Alanine









Aliphatic Amino Acids:

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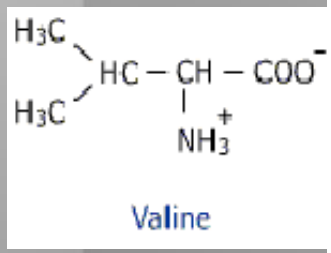
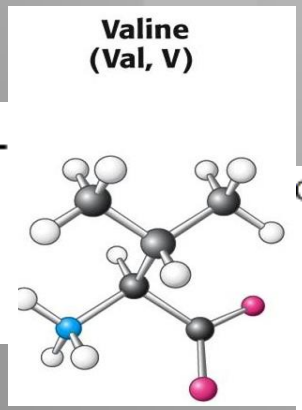
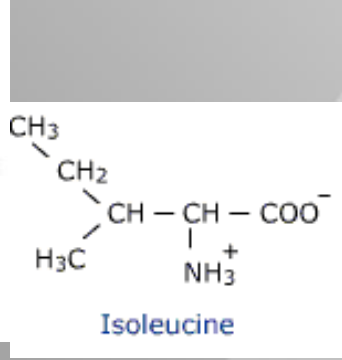
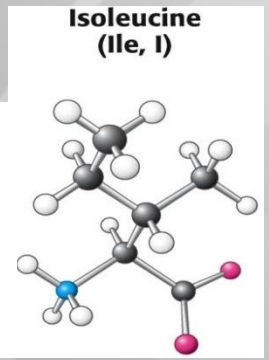
a) Mono-amino mono-carboxylic acids:

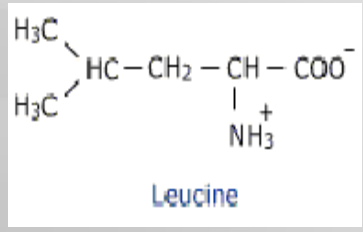
- Branched chain amino acids: Valine, Leucine and Isoleucine

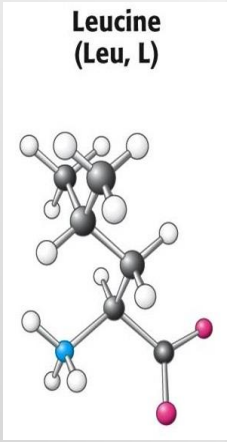












Aliphatic Amino Acids:

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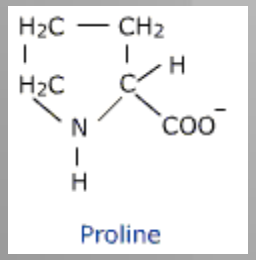
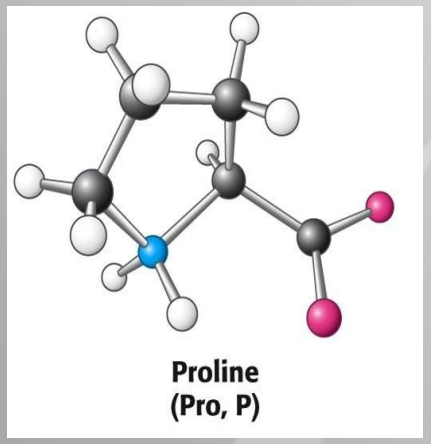
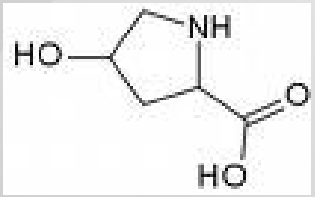
iv) Imino acid- Proline





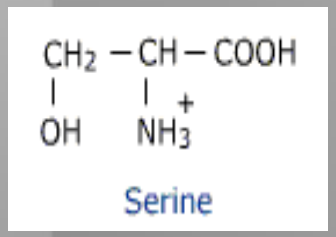


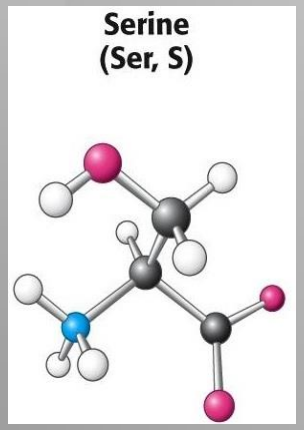
Polar Amino Acids:

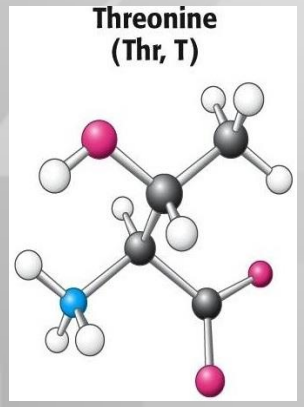
The University of Georgia

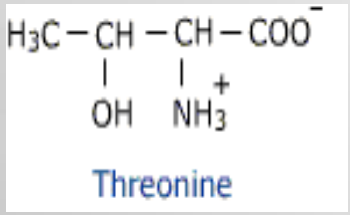
a) Mono-amino mono-carboxylic acids:

- -OH group-containing amino acids: Serine and Threonine









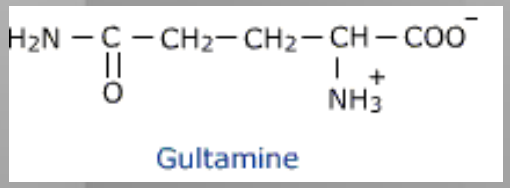
Polar Amino Acids:

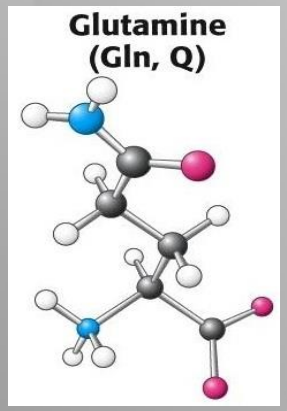
The University of Georgia

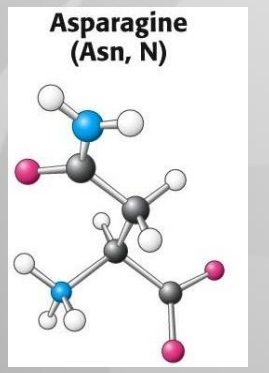
a) Mono-amino mono-carboxylic acids:

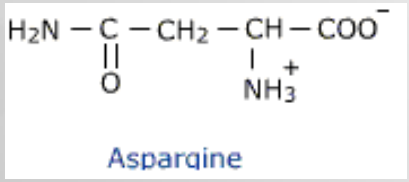
- ❑ Amide group-containing amino acids:

Glutamine and Asparagine







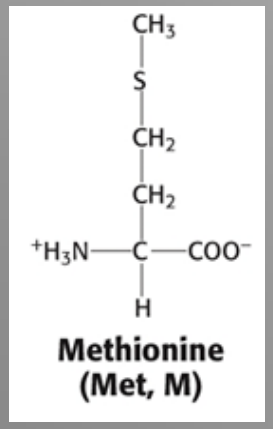


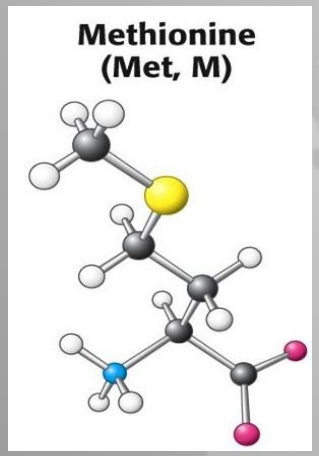
Non-Polar Amino Acids:

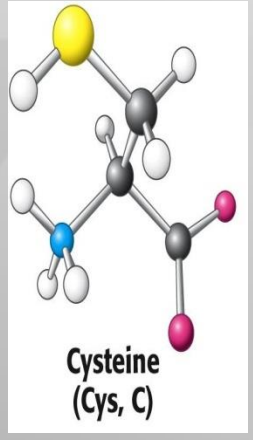
The University of Georgia

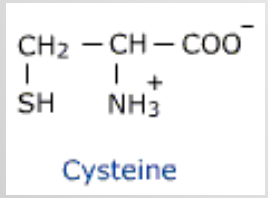
a) Mono-amino mono-carboxylic acids:

- Sulfur-containing amino acids: Cysteine, Cystine(Formed by linking of two cysteine residues) and Methionine.





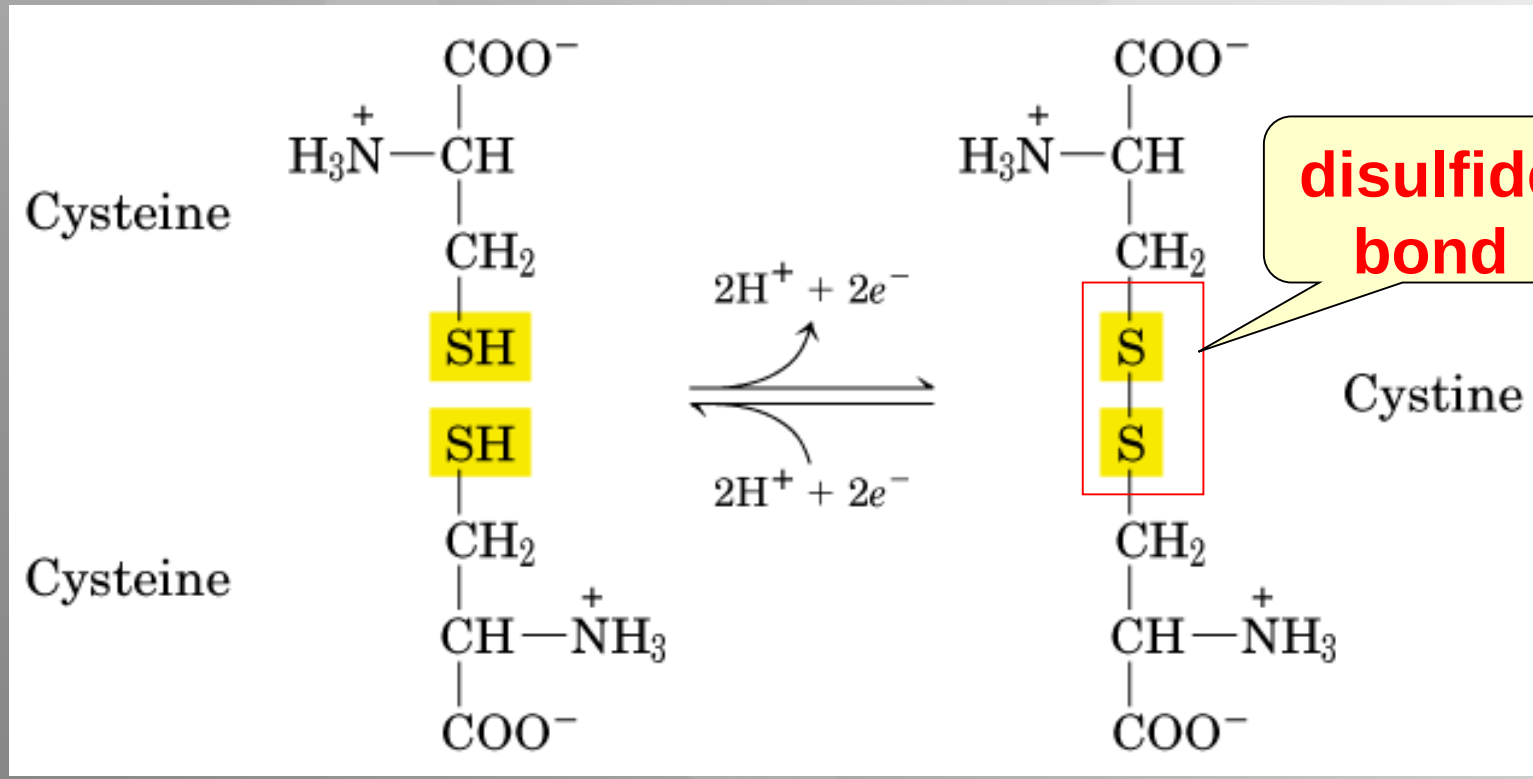




➢Disulfide bonds

➢-SH group of two Cys in proteins can be ***oxidized to form a covalent disulfide bond.***

➢ **Disulfide bonds: play a special role in the structures of many proteins by forming covalent links.**



Polar Amino Acids:

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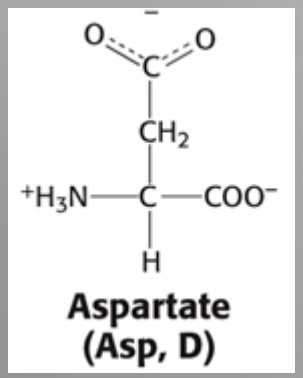
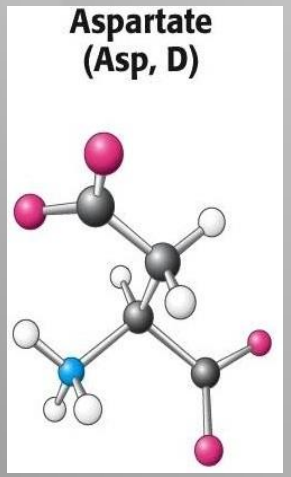
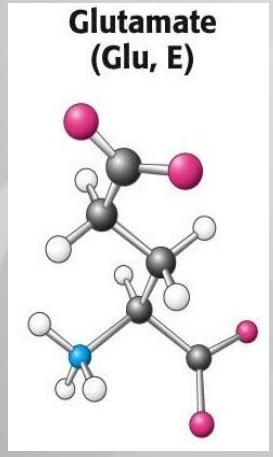
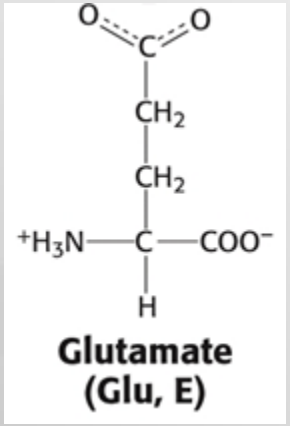
b) Mono-amino di-carboxylic acids: Aspartic acid and Glutamic acid









Polar Amino Acids:

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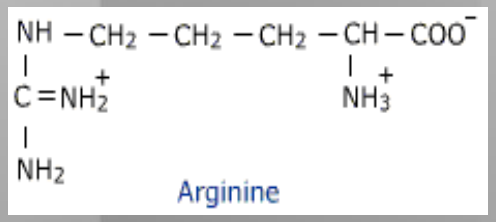
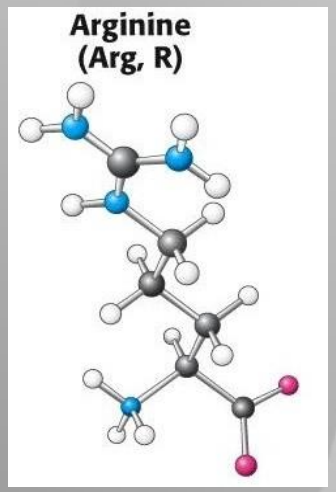
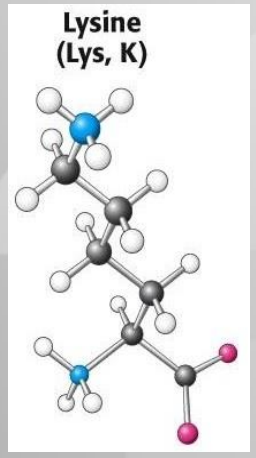
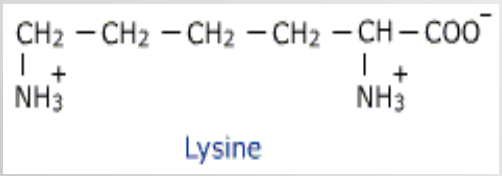
c) Di- basic mono-carboxylic acids: Arginine and Lysine









Polar Amino Acids:

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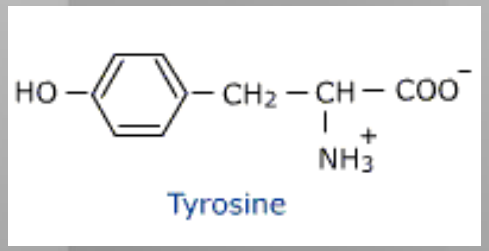
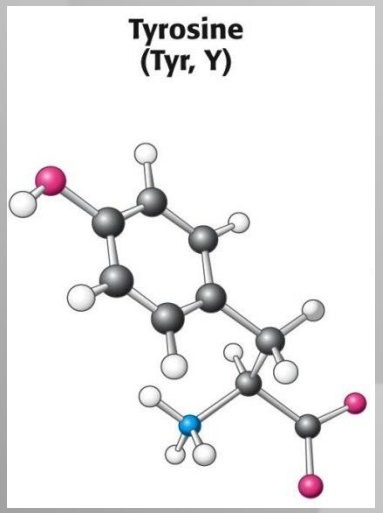
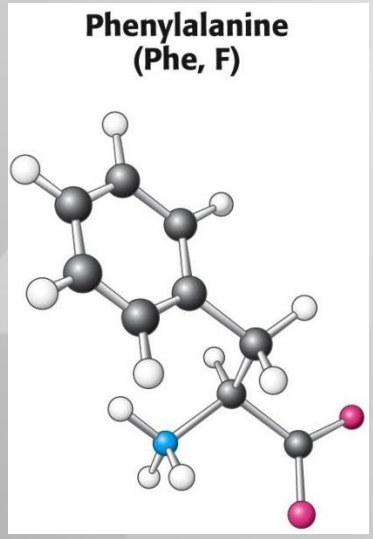
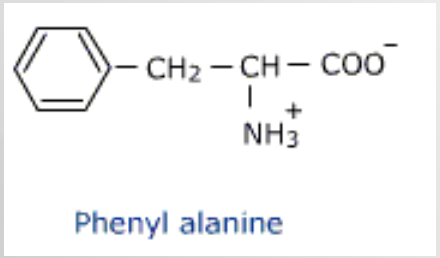
a-3) Aromatic amino acids-

- Phenyl alanine and tyrosine









Aromatic amino acids

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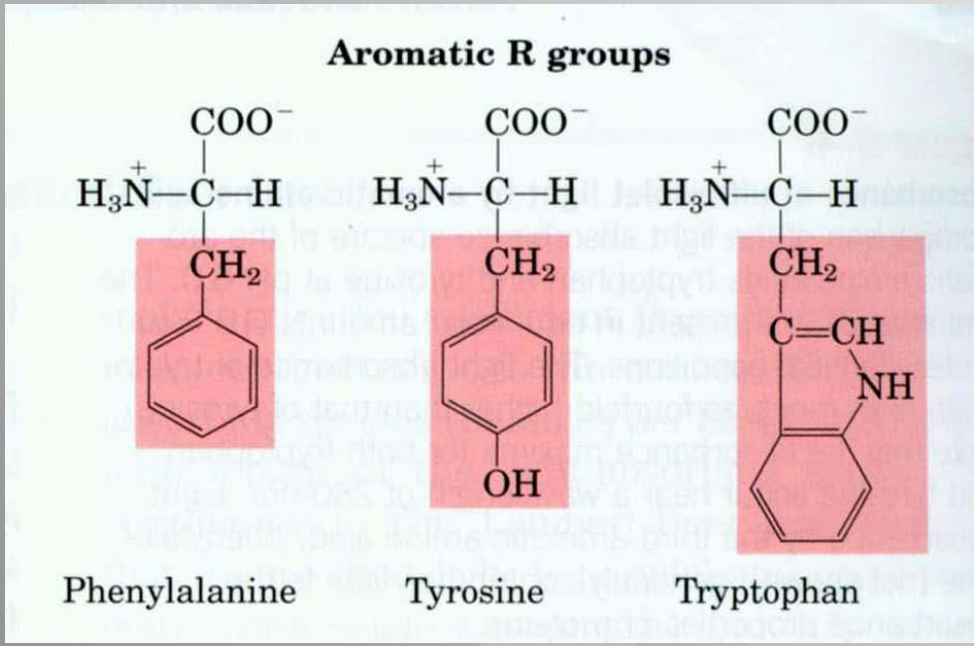
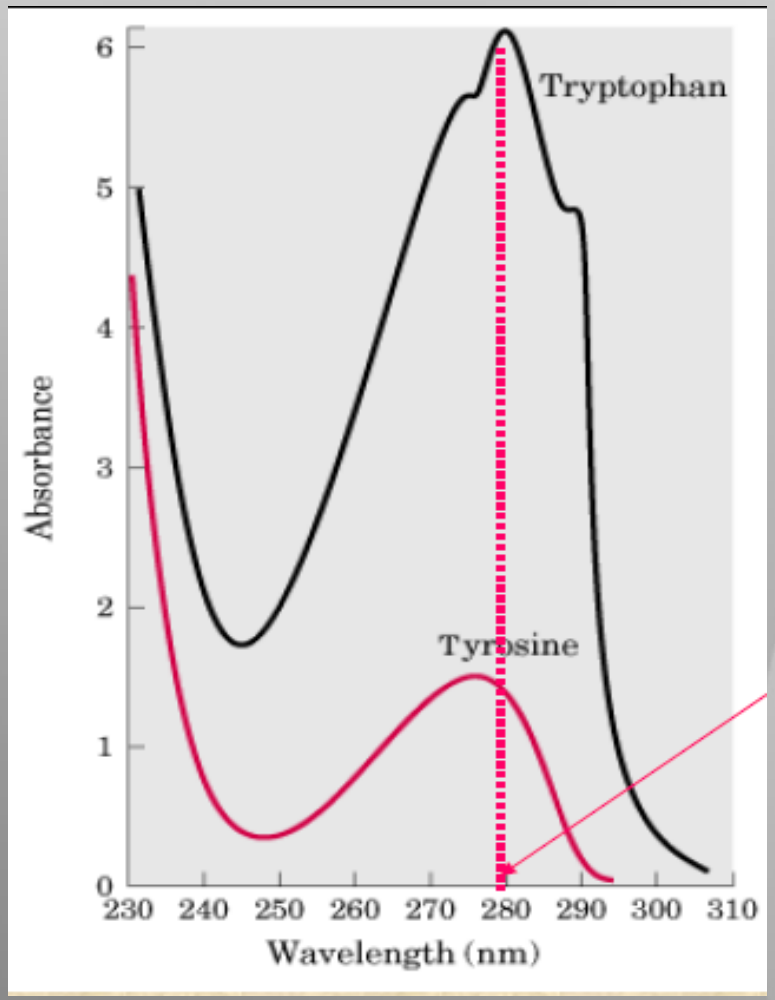
- **Phe, Tyr and Trp.**
  - **Phe and Tyr: benzene rings.**
  - **Tryptophan: indole ring.**



- **The -OH group in Tyr is an important functional group in proteins. (phosphorylation, hydrogen bond, etc), polar**

•**They are jointly responsible for the light absorption of proteins at 280 nm.**

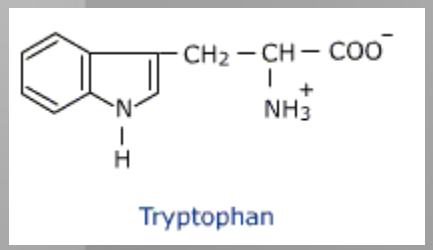


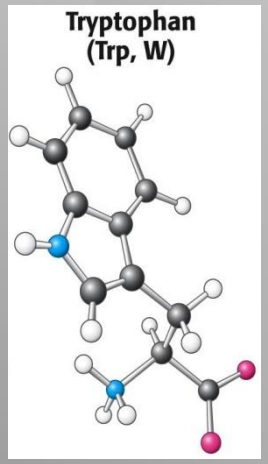
- Proteins in solution absorb UV light with absorbance maximum at 280nm.
- Measuring protein content by photo spectrometry.

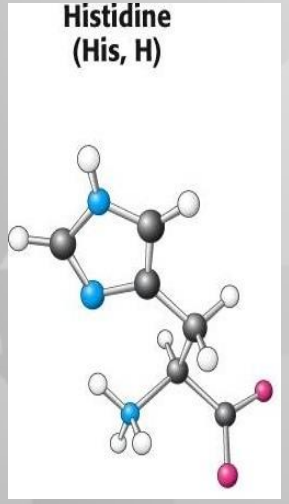
Polar Amino Acids:

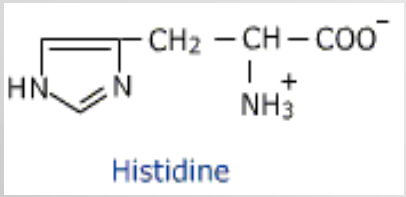
The University of Georgia

a-4) Heterocyclic Amino Acids: Tryptophan and Histidine









Acidic amino acids

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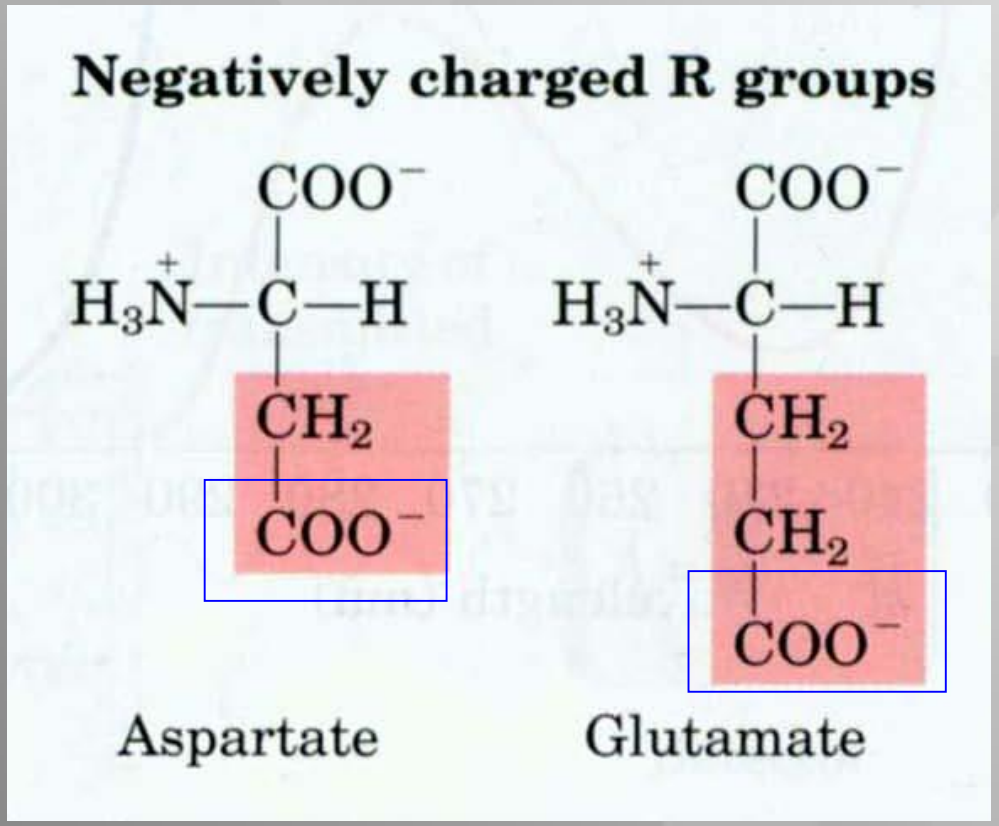
- Asp and Glu
  - Have carboxyl in their R groups.



Basic amino acids

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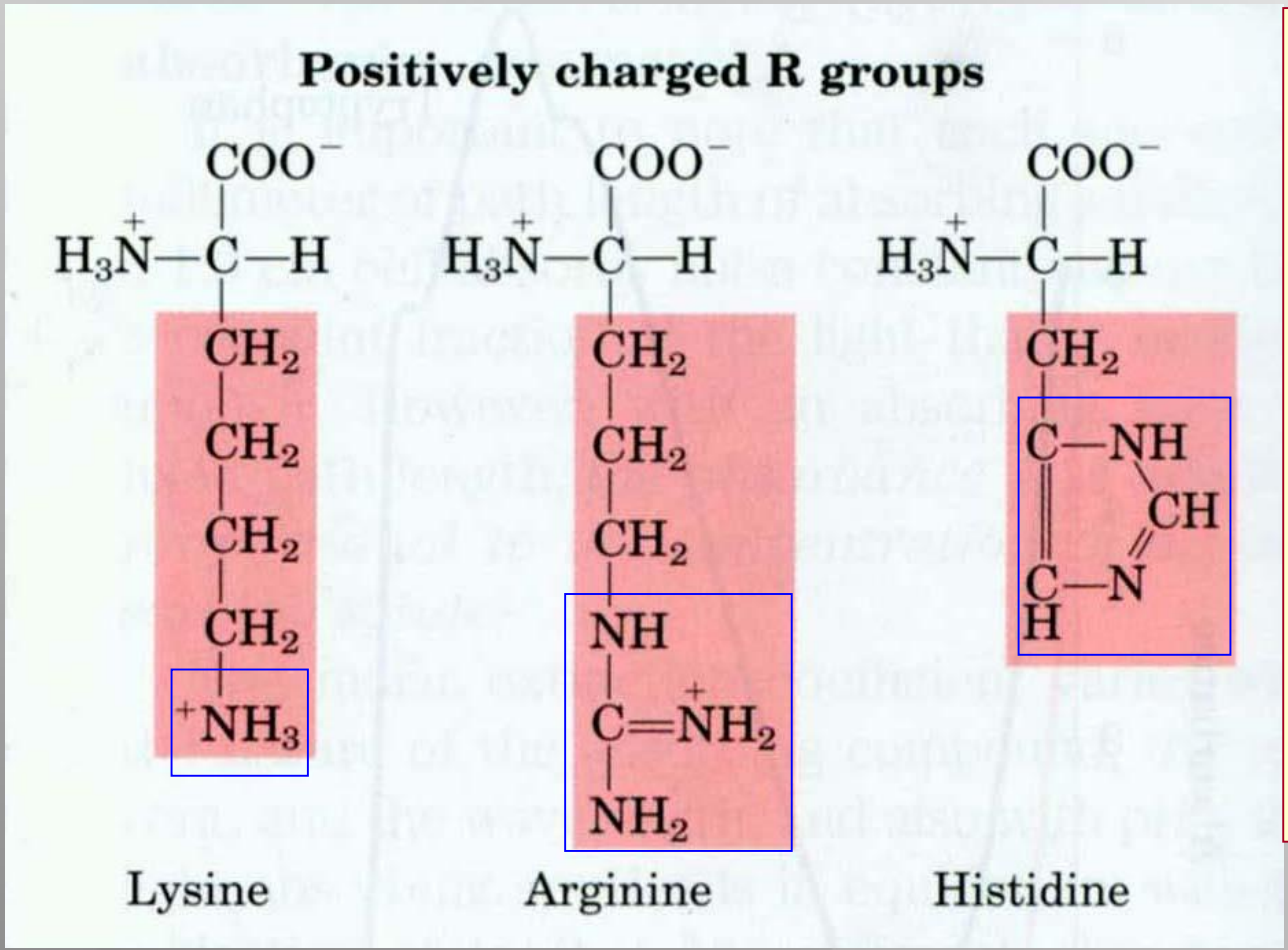
- Lys, Arg, and His.



- R groups
  - Amino
  - Guanidino
  - Imidazole
- Positive charged R groups at pH 7.0

- **Note these structural features**

1. All 20 are α-amino acids
2. For 19 of the 20, the α -amino group is primary; for proline, it is secondary (imino acid)
3. Except glycine, the α -carbons for 19 of them are asymmetric (or chiral).

- **Nonpolar Amino Acids**

Ala Val Leu Ile Gly Pro Phe Trp

- **Polar,Uncharged Amino Acids**

Ser Thr Cys Asn Gln Met Tyr

Aromatic

- **Acidic Amino Acids** Asp Glu

- **Basic Amino Acids** Lys Arg His

Nonstandard amino acids

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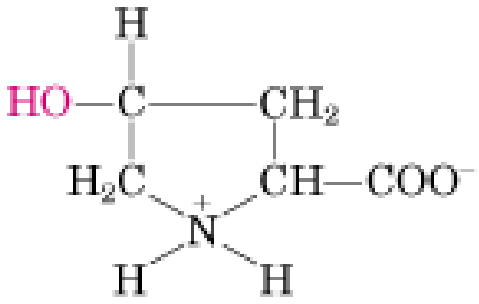
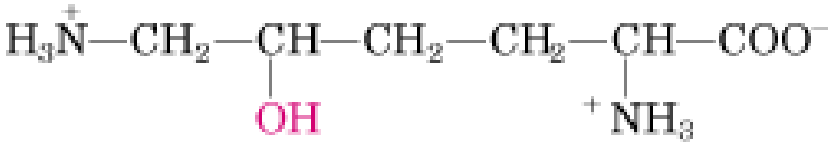
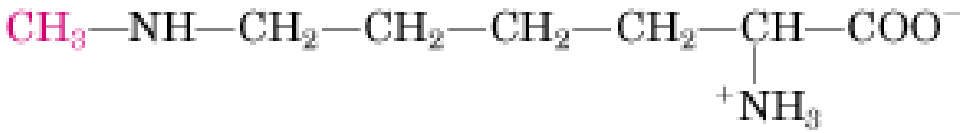
- **Amino acid derivatives found in proteins**
  - 4-Hydroxyproline **and 5-hydroxylysine in collagen.**
  - **6-*N*-Methyllysine in myosin.**



4-Hydroxyproline

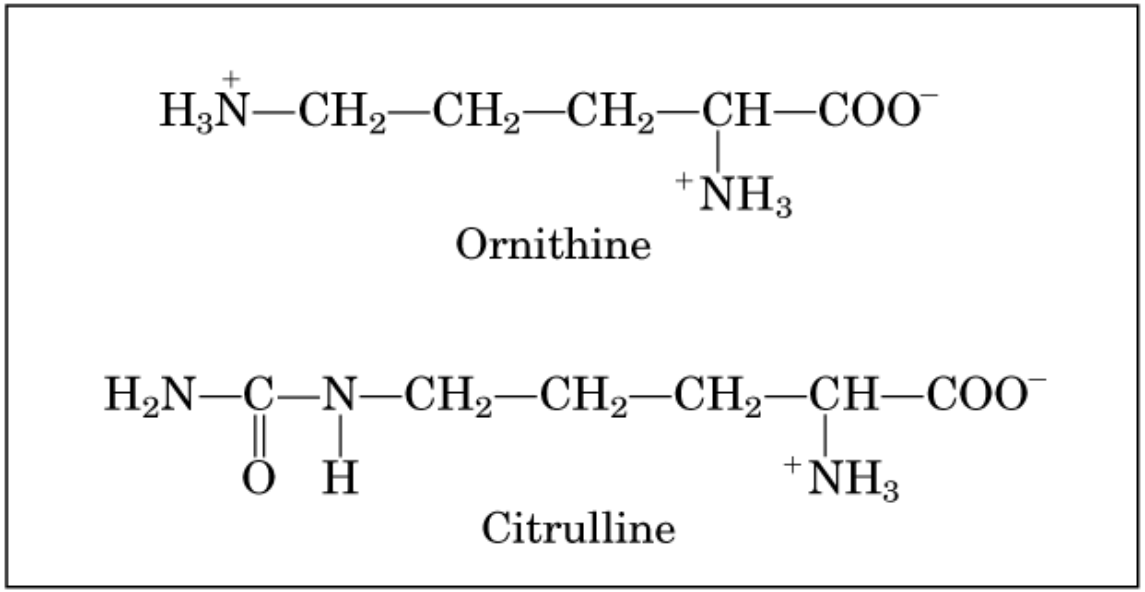


5-Hydroxylysine



6-*N*-Methyllysine

Many additional nonstandard amino acids are found in cells, but not in proteins



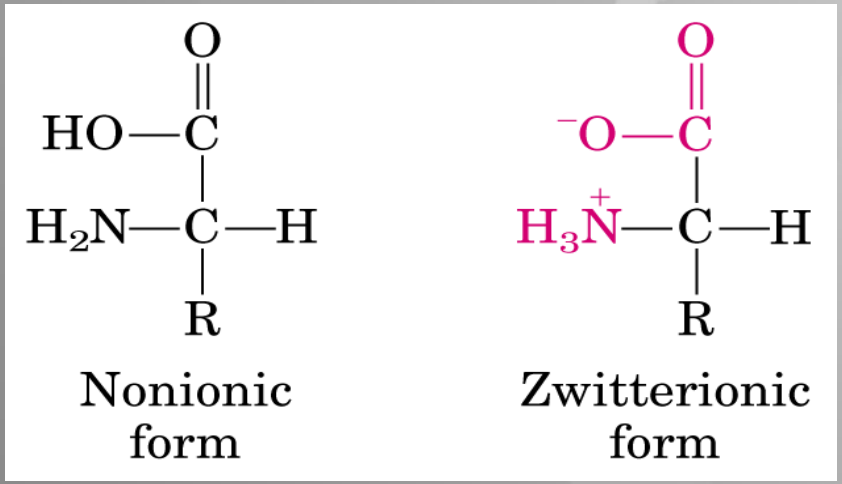
- Ornithine and citrulline
- Intermediates in amino acid metabolism.

Essential and non-essential amino acids

- Essential amino acids (or indispensable amino acids):
  - Cannot be synthesized by the humans, must be supplied in the diet
  - 8: Phe, Val, Thr, Trp, Ile, Met, Leu, Lys
- Semi-essential amino acids:
  - 2: His and Arg
  - Required by infants and growing children

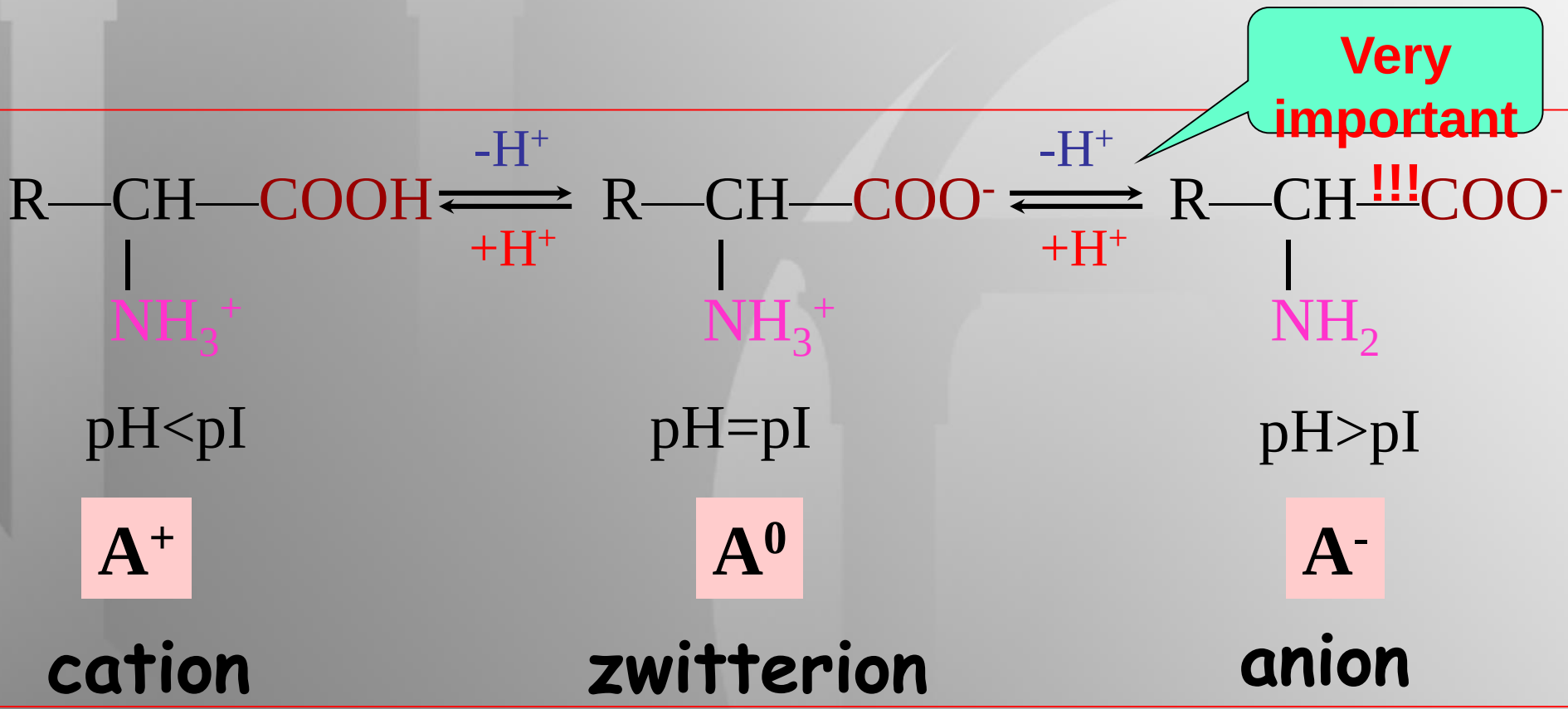
Acid/base properties of AAs *(Very important!)*

- Amino acid has both a basic amine group and an acidic carboxylic acid group.
- In neutral solution (pH 7.0), the amino acid contains a negative charge and a positive charge. It is called a *zwitterion* (German for "hybrid ion").



•AAs ionize to various states depending on pH values.

• pI: there is a specific pH (designated isoelectric point, pI) at which an AA has equal positive and negative charge (no net electric charge) .



Properties and Conventions Associated with the Standard Amino Acids

Amino acid	Abbreviated names		M_r	pK_a values: pK_1 (—COOH)	pK_2 ($—NH_3^+$)	pK_R (R group)	pI	Hydropathy index*	Occurrence in proteins (%)†
Nonpolar, aliphatic R groups									
Glycine	Gly	G	75	2.34	9.60		5.97	−0.4	7.2
Alanine	Ala	A	89	2.34	9.69		6.01	1.8	7.8
Valine	Val	V	117	2.32	9.62		5.97	4.2	6.6
Leucine	Leu	L	131	2.36	9.60		5.98	3.8	9.1
Isoleucine	Ile	I	131	2.36	9.68		6.02	4.5	5.3
Methionine	Met	M	149	2.28	9.21		5.74	1.9	2.3
Aromatic R groups									
Phenylalanine	Phe	F	165	1.83	9.13		5.48	2.8	3.9
Tyrosine	Tyr	Y	181	2.20	9.11	10.07	5.66	−1.3	3.2
Tryptophan	Trp	W	204	2.38	9.39		5.89	−0.9	1.4
Polar, uncharged R groups									
Serine	Ser	S	105	2.21	9.15		5.68	−0.8	6.8
Proline	Pro	P	115	1.99	10.96		6.48	1.6	5.2
Threonine	Thr	T	119	2.11	9.62		5.87	−0.7	5.9
Cysteine	Cys	C	121	1.96	10.28	8.18	5.07	2.5	1.9
Asparagine	Asn	N	132	2.02	8.80		5.41	−3.5	4.3
Glutamine	Gln	Q	146	2.17	9.13		5.65	−3.5	4.2
Positively charged R groups									
Lysine	Lys	K	146	2.18	8.95	10.53	9.74	−3.9	5.9
Histidine	His	H	155	1.82	9.17	6.00	7.59	−3.2	2.3
Arginine	Arg	R	174	2.17	9.04	12.48	10.76	−4.5	5.1
Negatively charged R groups									
Aspartate	Asp	D	133	1.88	9.60	3.65	2.77	−3.5	5.3
Glutamate	Glu	E	147	2.19	9.67	4.25	3.22	−3.5	6.3

Polypeptides

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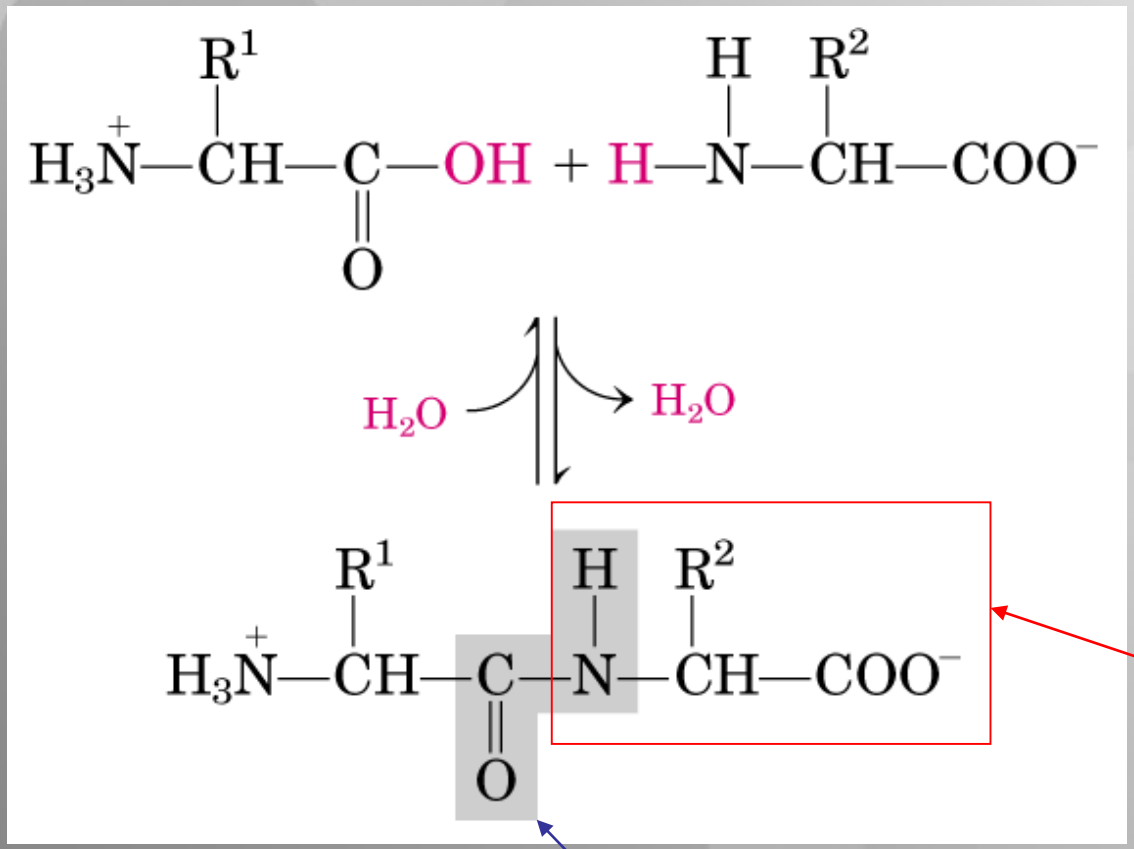
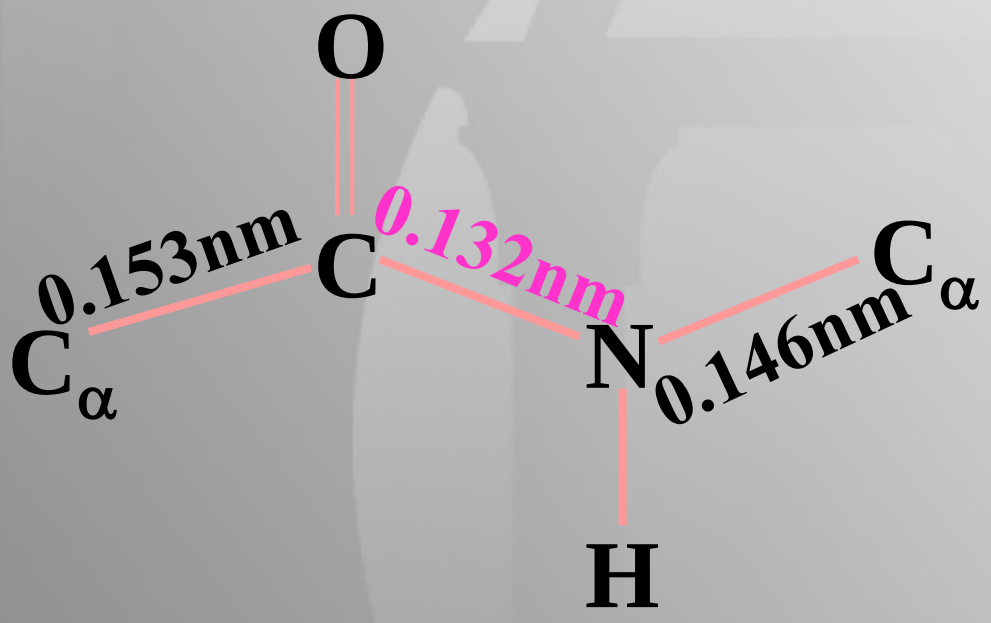
Peptide bond: the special name given to the amide bond between the carboxyl group of one amino acid and the -amino group of another.

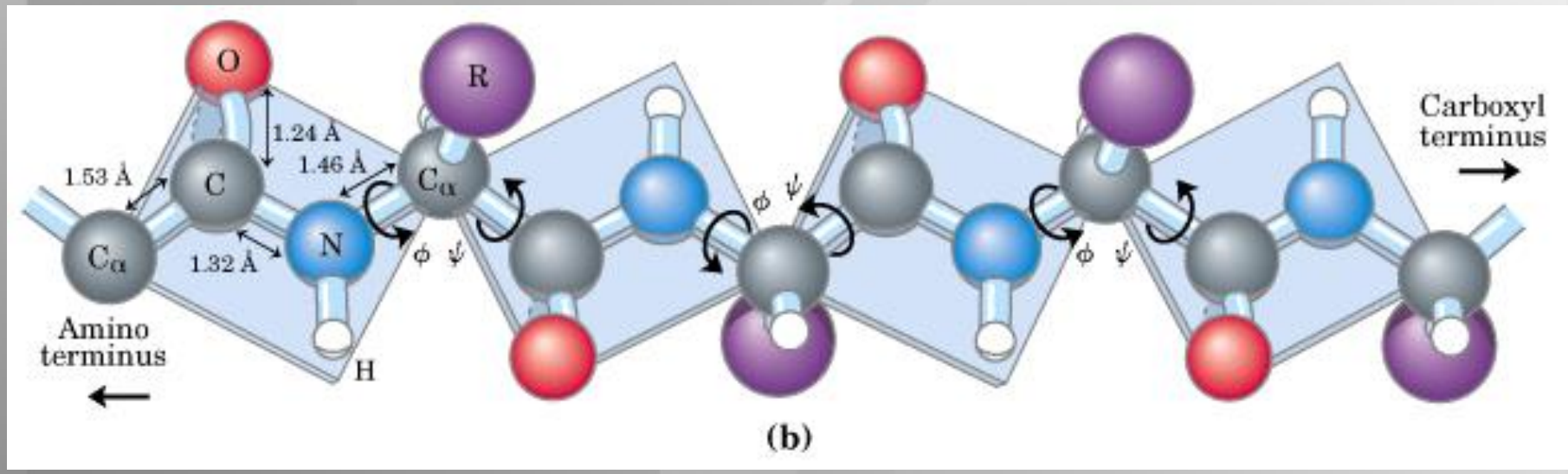


Characteristics of the peptide bond

- The peptide bond have partial double bond feature
  - about 0.132nm (C-N single bond, 0.149nm; C=N double bond, 0.127nm),
  - *rigid and unable to rotate freely*.



- The peptide bond is planar, trans-configuration and uncharged.
- Peptide plane: the six atoms attached to the peptide bond are coplanar.
- the carbonyl oxygen and the amide hydrogen are in trans positions.



The peptide chain is directional.

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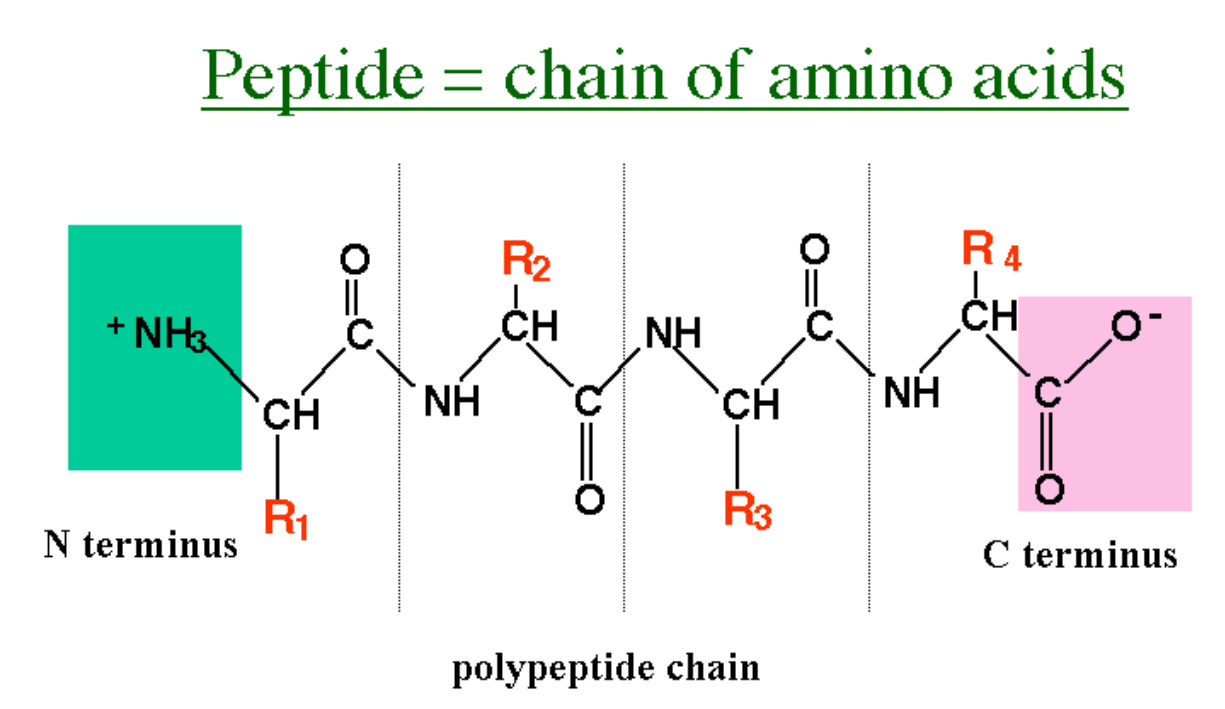
- Amino-terminal or N-terminal: the end having a free a-amino group.
- Carboxyl-terminal or C-terminal: the end having a free a-carboxyl group.
- By convention, the N-terminal is taken as the beginning of the peptide chain, and put at the left (C-terminal at the right).

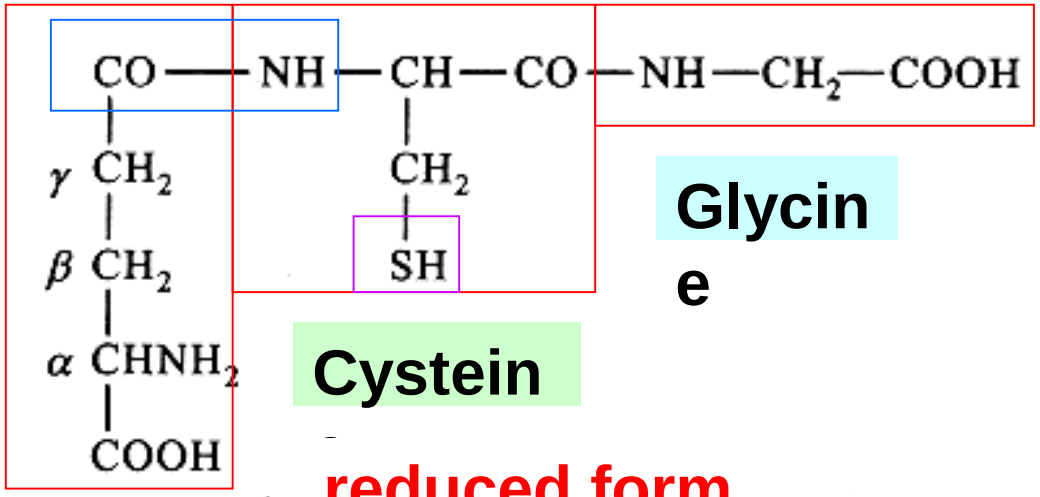


Polymers of amino acids

- Peptides can be classified according to how many amino acids they contain
  - Dipeptide: 2 amino acid residues, tripeptide: 3 residues, and so on
  - Oligopeptide: 12~20 residues
  - Polypeptide: many residues

Biologically important peptide

- Glutathione (GSH)
  - Tripeptide: glutamic acid, cysteine and glycine;
  - Function: important in biological oxidation-reduction reactions, has reduced and oxidized form.
  - It's the most important molecule you need to stay healthy and prevent disease.

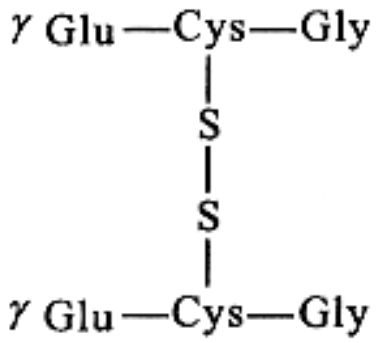


Glycin
e

Cystein

Glutamic

reduced form
GSH



- oxidized form glutathione


TIME
FOR A
BREAK

PDB

- Protein databank
- 162,269 entries (4/6/2020)

PDB Format

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- The PDB format consists of a collection of fixed format records that describe :
  - Atomic coordinates,
  - Chemical and biochemical features
  - Experimental details of the structure determination
  - Some structural features such as
    - Secondary structure assignments,
    - Hydrogen bonding
    - Biological assemblies
    - Active sites

PDB Format

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```
SHEET    3   L 3 THR H 212  VAL H 214 -1  O  THR H 212   N  HIS H 207
SHEET    1   M 3 THR H 158  TRP H 161  0
SHEET    2   M 3 TYR H 201  HIS H 207 -1  O  ASN H 206   N  THR H 158
SHEET    3   M 3 LYS H 217  VAL H 218 -1  O  VAL H 218   N  TYR H 201
SHEET    1   N 3 TRP C  28  LEU C  29  0
SHEET    2   N 3 VAL C  13  ALA C  18 -1  N  VAL C  17   O  LEU C  29
SHEET    3   N 3 LEU C  36  ALA C  38 -1  O  LEU C  36   N  HIS C  15
SHEET    1   O 5 TRP C  28  LEU C  29  0
SHEET    2   O 5 VAL C  13  ALA C  18 -1  N  VAL C  17   O  LEU C  29
SHEET    3   O 5 TYR C 151  ALA C 156 -1  O  ILE C 154   N  ALA C  14
SHEET    4   O 5 GLY C  54  GLN C  67 -1  N  TYR C  59   O  GLY C 153
SHEET    5   O 5 PRO C 113  LEU C 126 -1  O  GLY C 122   N  ILE C  58
SHEET    1   P 5 GLU C  42  ARG C  44  0
SHEET    2   P 5 GLN C  47  VAL C  49 -1  O  VAL C  49   N  GLU C  42
SHEET    3   P 5 ARG C 131  ILE C 136 -1  O  LEU C 132   N  LEU C  48
SHEET    4   P 5 LEU C  76  ILE C  83 -1  N  THR C  79   O  GLU C 135
SHEET    5   P 5 LYS C  90  LYS C  98 -1  O  LEU C  94   N  ILE C  80
SSBOND   1 CYS L   23    CYS L   88                          1555   1555  2.05
SSBOND   2 CYS L  134    CYS L  194                          1555   1555  2.03
SSBOND   3 CYS H   22    CYS H   98                          1555   1555  2.05
SSBOND   4 CYS H  147    CYS H  203                          1555   1555  2.03
SSBOND   5 CYS C   69    CYS C  101                          1555   1555  2.06
CISPEP   1 SER L    7    PRO L    8          0         2.35
CISPEP   2 TRP L   94    PRO L   95          0         6.74
CISPEP   3 TYR L  140    PRO L  141          0         1.27
CISPEP   4 GLU H    1    VAL H    2          0         3.36
CISPEP   5 GLY H  140    GLY H  141          0         9.68
CISPEP   6 PHE H  153    PRO H  154          0        -3.35
CISPEP   7 GLU H  155    PRO H  156          0         0.91
CISPEP   8 CYS C  101    GLN C  102          0        -3.69
CRYST1  153.663  153.663   99.279  90.00  90.00 120.00 H 3           9
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.006508  0.003757  0.000000        0.00000
SCALE2      0.000000  0.007514  0.000000        0.00000
SCALE3      0.000000  0.000000  0.010073        0.00000
ATOM      1  N   ASP L   1      24.141  -2.203  -3.932  1.00 34.47           N
ATOM      2  CA  ASP L   1      25.160  -2.458  -2.905  1.00 44.54           C
ATOM      3  C   ASP L   1      25.772  -1.169  -2.301  1.00 43.71           C
```

how file was produced

the 17 numbered atoms

coordinates

```
HEADER
REMARK Spartan ST exported MOO1      x       y       z
HETATM    1 Cu  UNK  0001        0.000   0.000   0.000
HETATM    2  N  UNK  0001       -0.870   0.000   1.728
HETATM    3  H  UNK  0001       -1.884   0.000   1.654
HETATM    4  H  UNK  0001       -0.607   0.825   2.263
HETATM    5  H  UNK  0001       -0.607  -0.825   2.263
HETATM    6  N  UNK  0001       -1.728   0.000  -0.870
HETATM    7  H  UNK  0001       -1.654   0.000  -1.884
HETATM    8  H  UNK  0001       -2.263   0.825  -0.607
HETATM    9  H  UNK  0001       -2.263  -0.825  -0.607
HETATM   10  N  UNK  0001        0.870   0.000  -1.728
HETATM   11  H  UNK  0001        1.884   0.000  -1.654
HETATM   12  H  UNK  0001        0.607   0.825  -2.263
HETATM   13  H  UNK  0001        0.607  -0.825  -2.263
HETATM   14  N  UNK  0001        1.728   0.000   0.870
HETATM   15  H  UNK  0001        1.654   0.000   1.884
HETATM   16  H  UNK  0001        2.263   0.825   0.607
HETATM   17  H  UNK  0001        2.263  -0.825   0.607
CONECT    1    2    6   10   14
CONECT    2    3    4    5    1
CONECT    3    2
CONECT    4    2
CONECT    5    2
CONECT    6    7    8    9    1
CONECT    7    6
CONECT    8    6
CONECT    9    6
CONECT   10   11   12   13    1
CONECT   11   10
CONECT   12   10
CONECT   13   10
CONECT   14   15   16   17    1
CONECT   15   14
CONECT   16   14
CONECT   17   14
END
```

How the 17 atoms are connected

PDB Format

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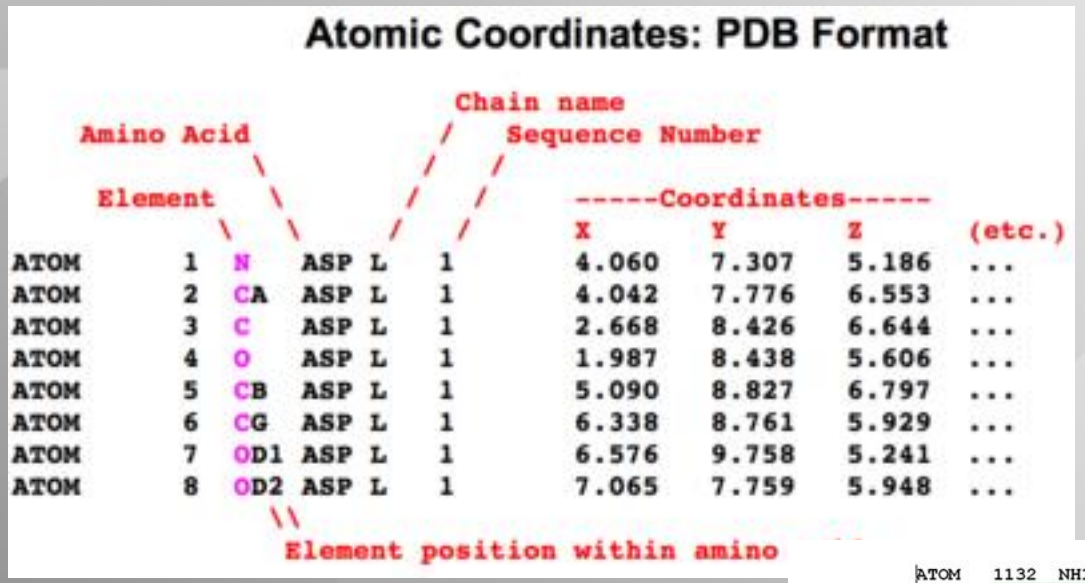

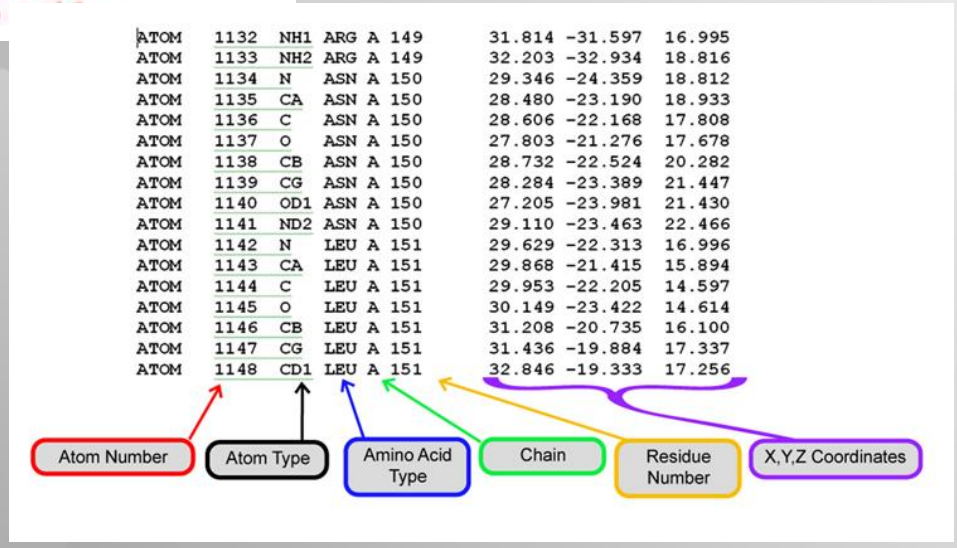

PDB Format

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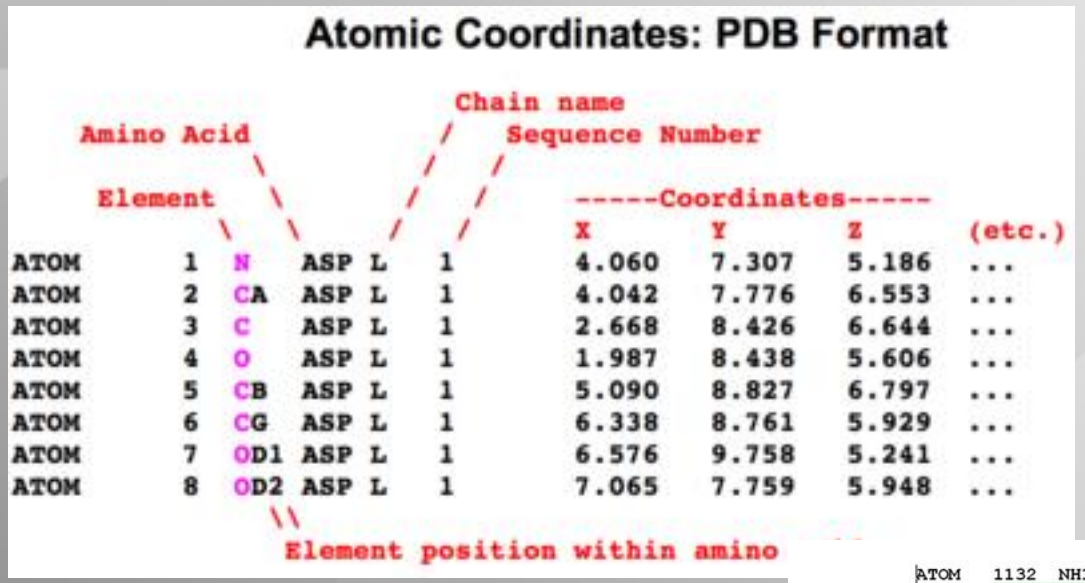

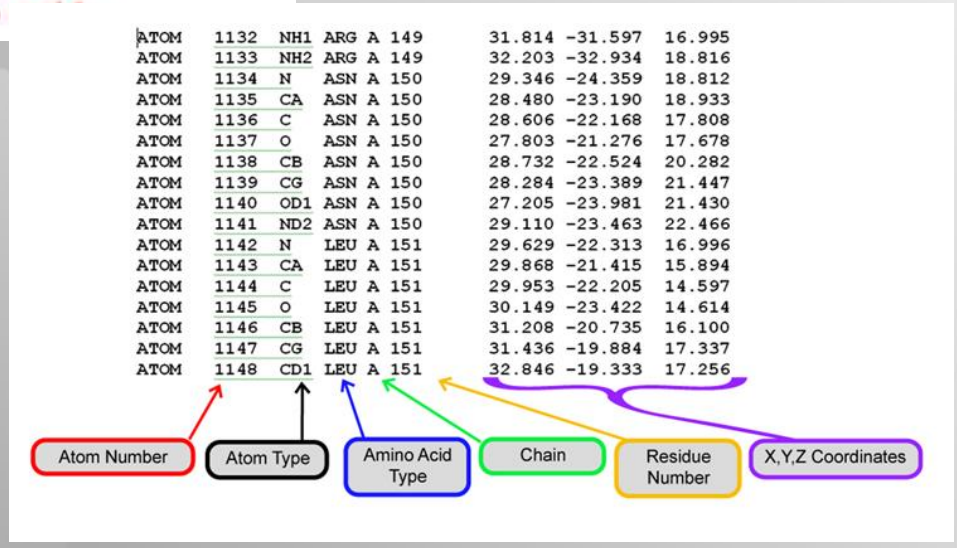

PDBsum

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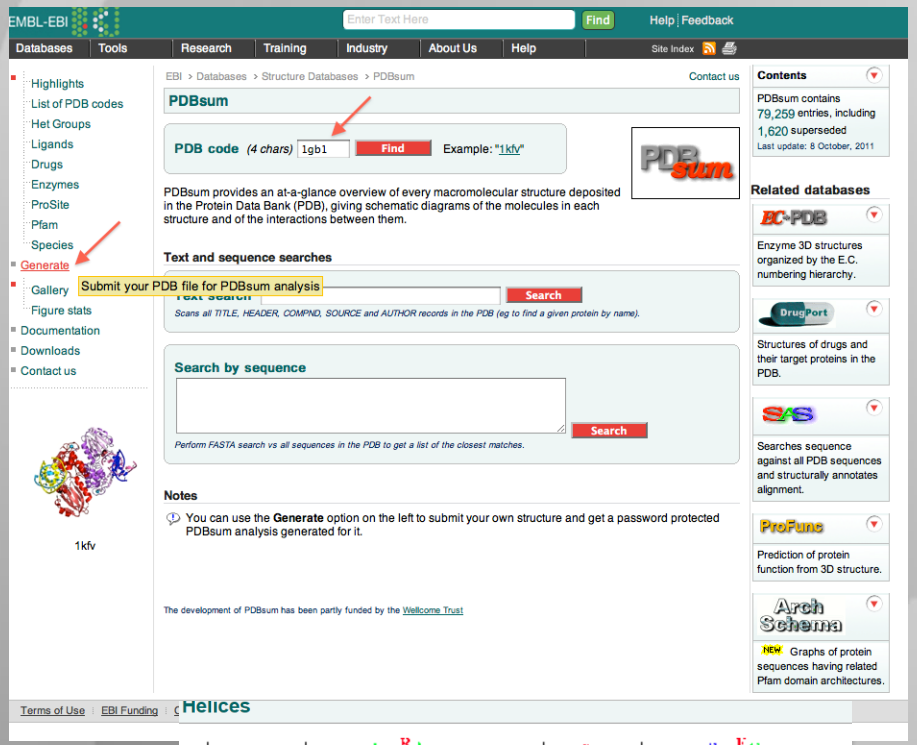

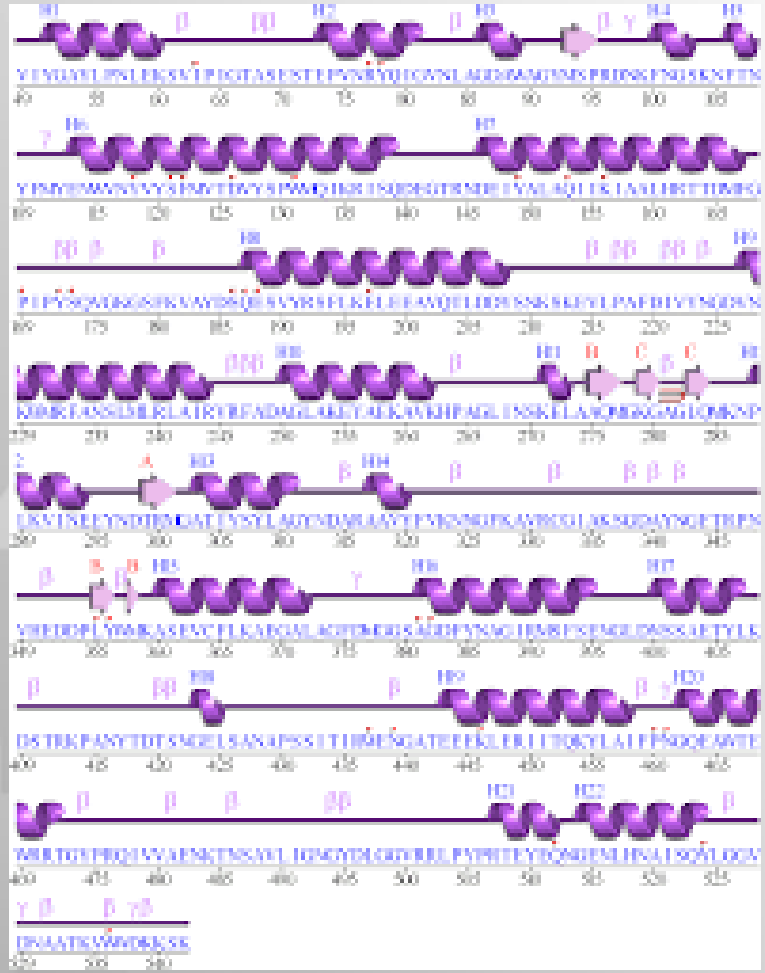

PDB

- Protein databank
- 126,978 entries

Software

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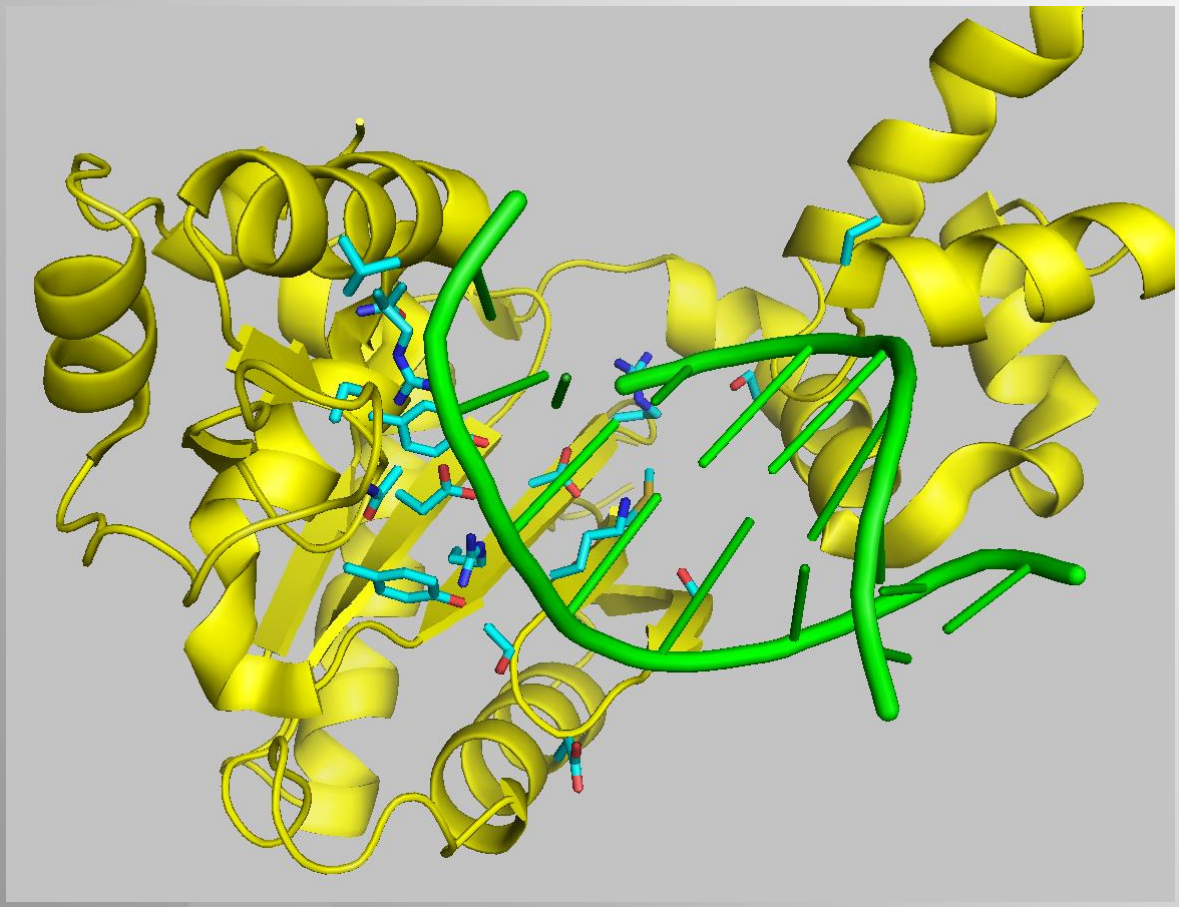
- VMD
- Pymol



Python Time

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