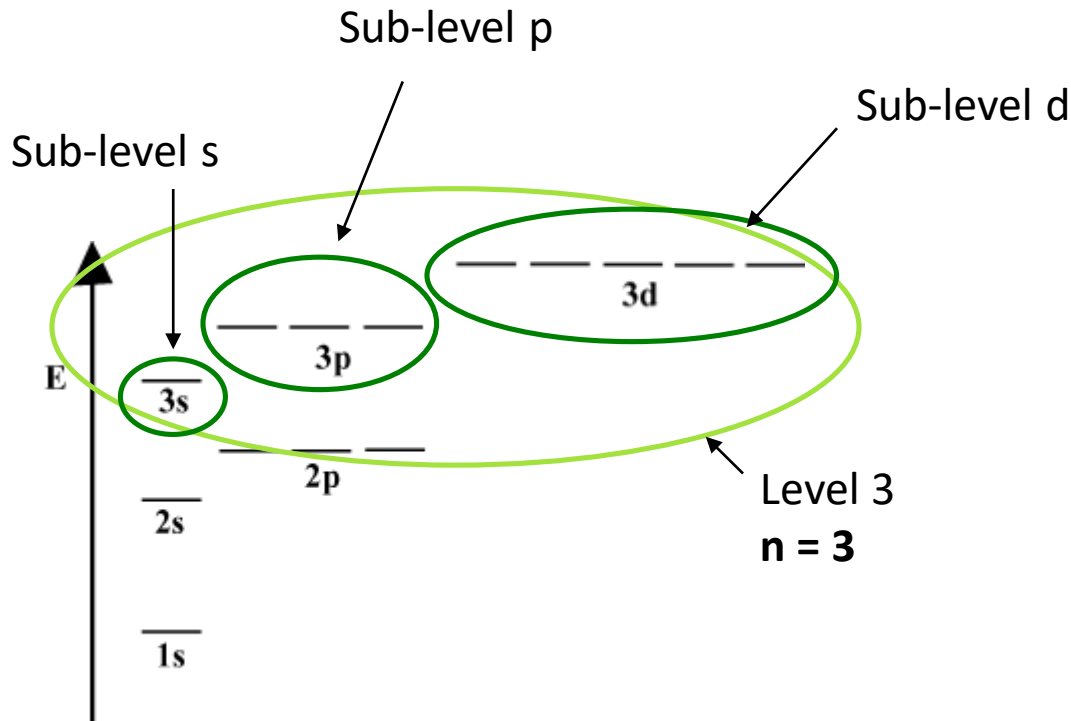




Chemistry of Life

Prof. Dr. Chiara Valsecchi

Atomic Orbitals Levels

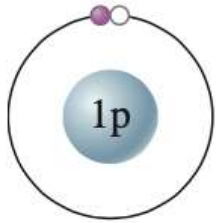
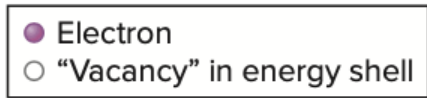


Each level can have sub-levels

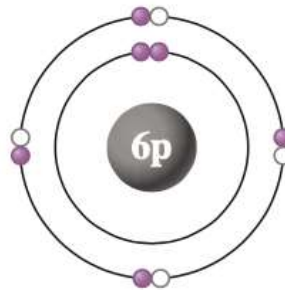
The outmost atomic orbital level is the one that will affect the capacity of the atoms to create bonds

VALENCE SHELL

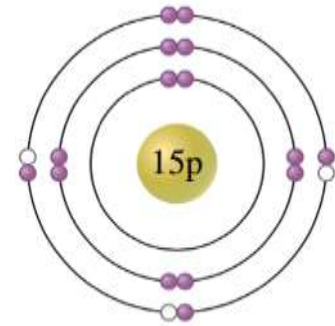
Valence Shell



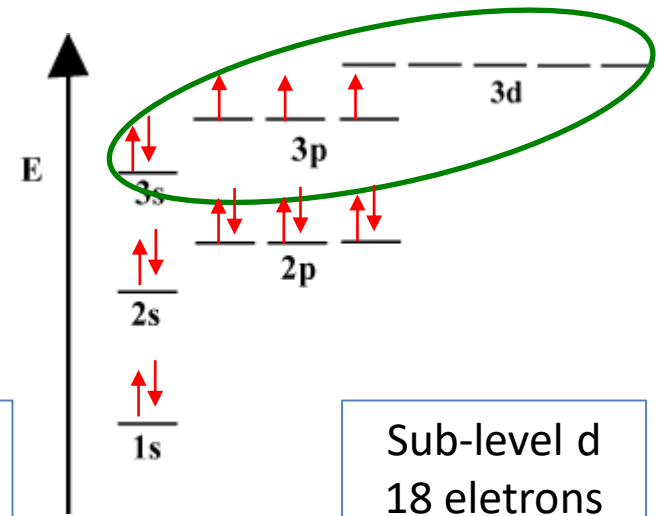
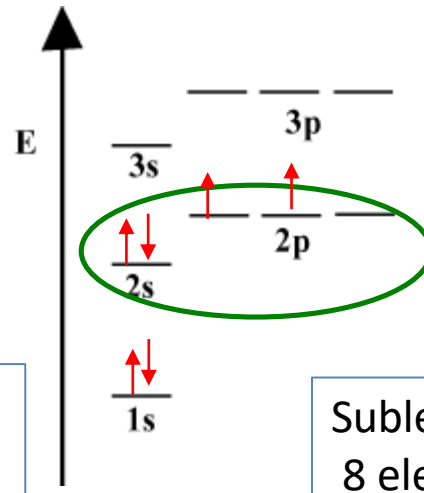
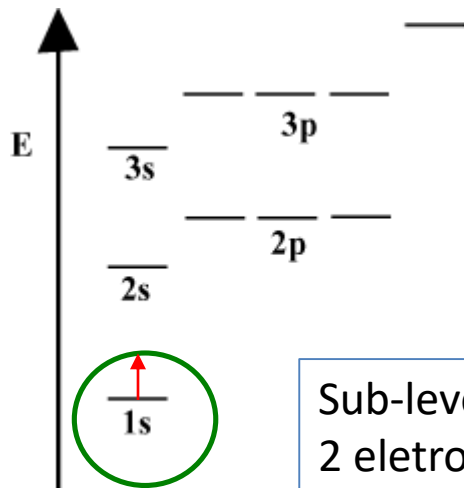
Hydrogen



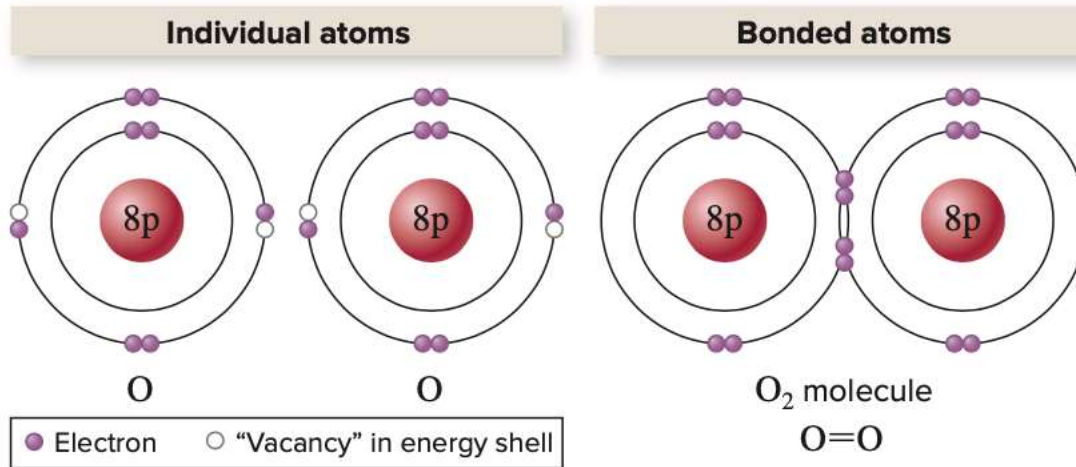
Carbon



Phosphorus



Covalent bond



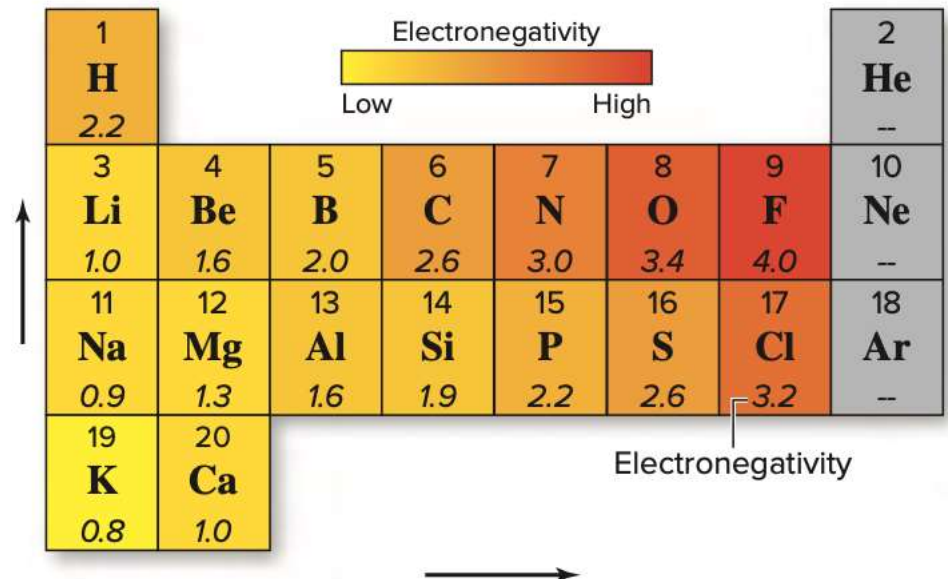
Electrons are shared

However, this is NOT
an equal sharing

Atoms that are more
electronegative (like O, F and Cl)
keep the electron more close

They have a partial negative
charge

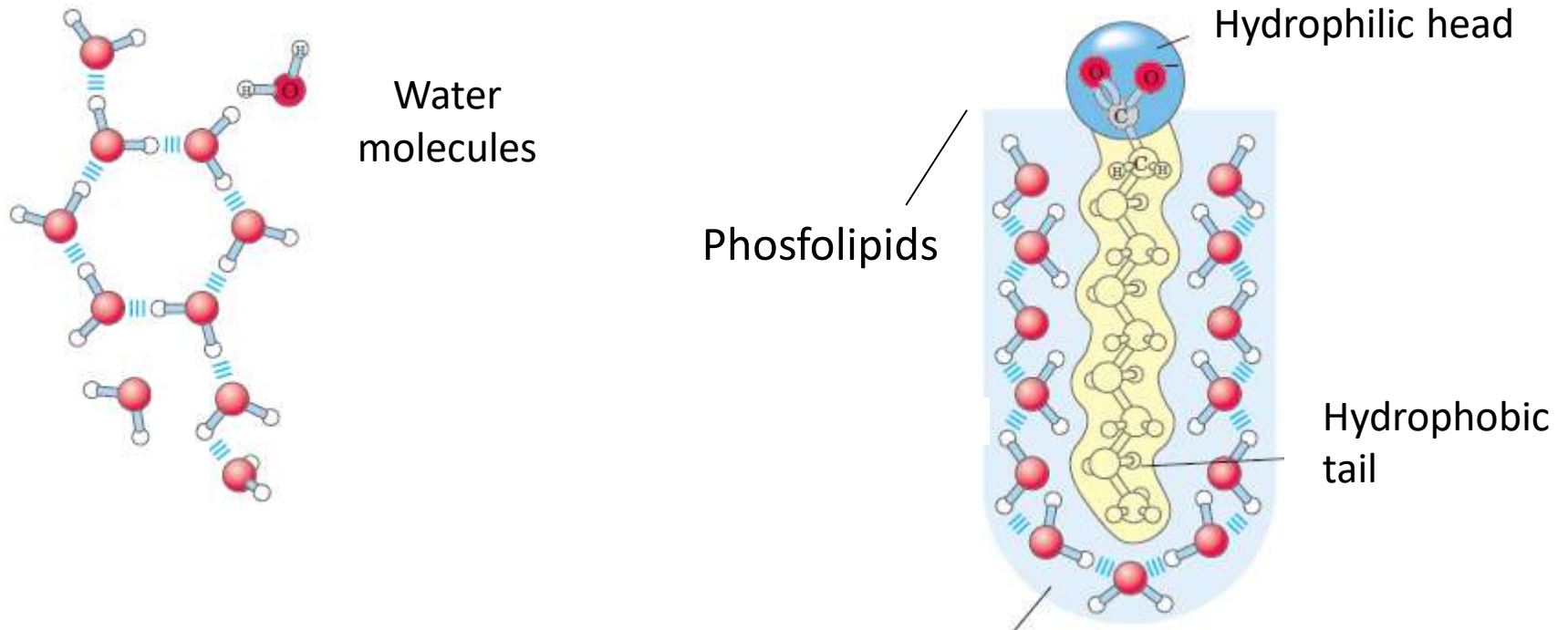
The others, a partial positive
charge



Polar or Apolar ?

Polar molecules interact between themselves and with water. They are called **HYDROPHILIC**.

Apolar molecules tend to separate from water (like oil): they are called **HYDROPHOBIC**.



pH Scale

Concentration of H^+ ions in water

To avoid scientific notation, due to small number, the pH Scale is actually a logarithmic scale

p : means: “minus logarithm of...”

Ex.:

$$[H^+] = 1,0 \times 10^{-5}$$

$$\text{pH} = -\log [H^+] = -\log [10^{-5}] = +5$$

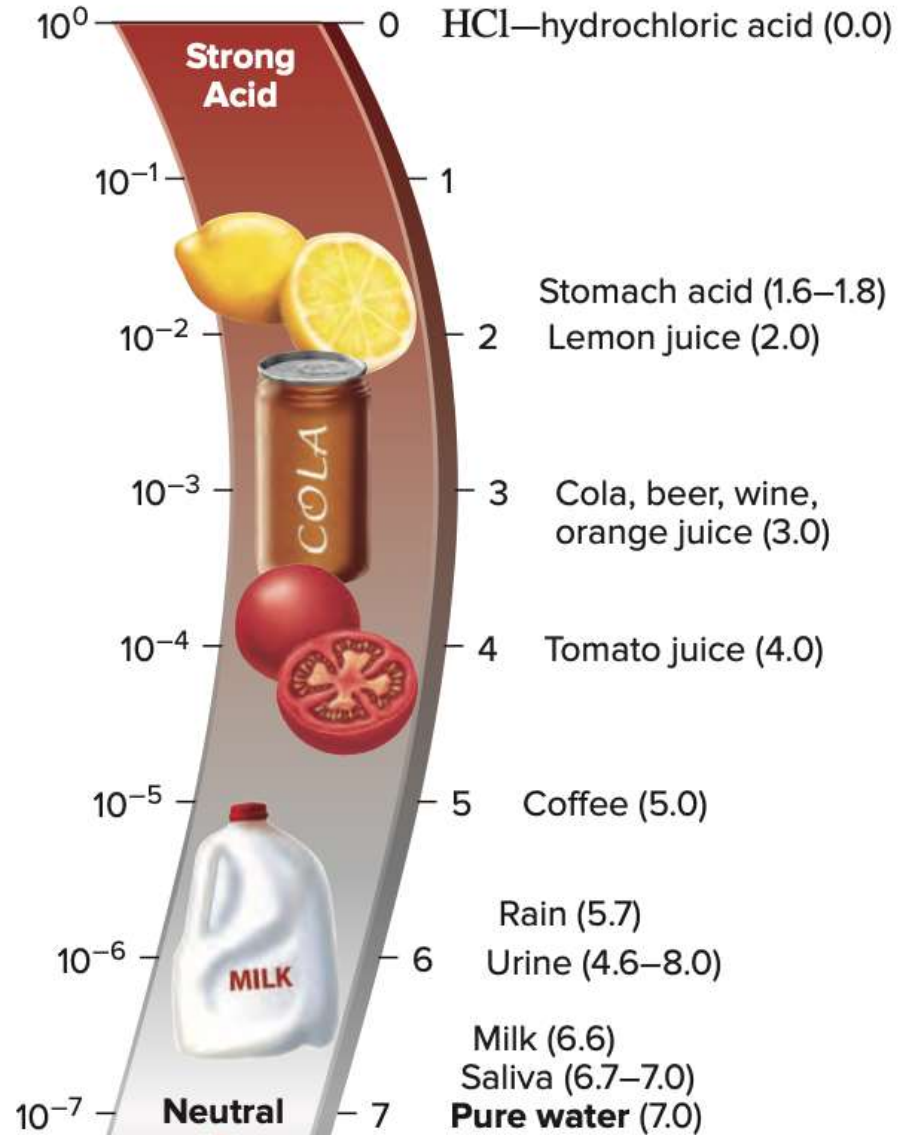
pH is negative logarithm of H^+ concentration

pH Scale

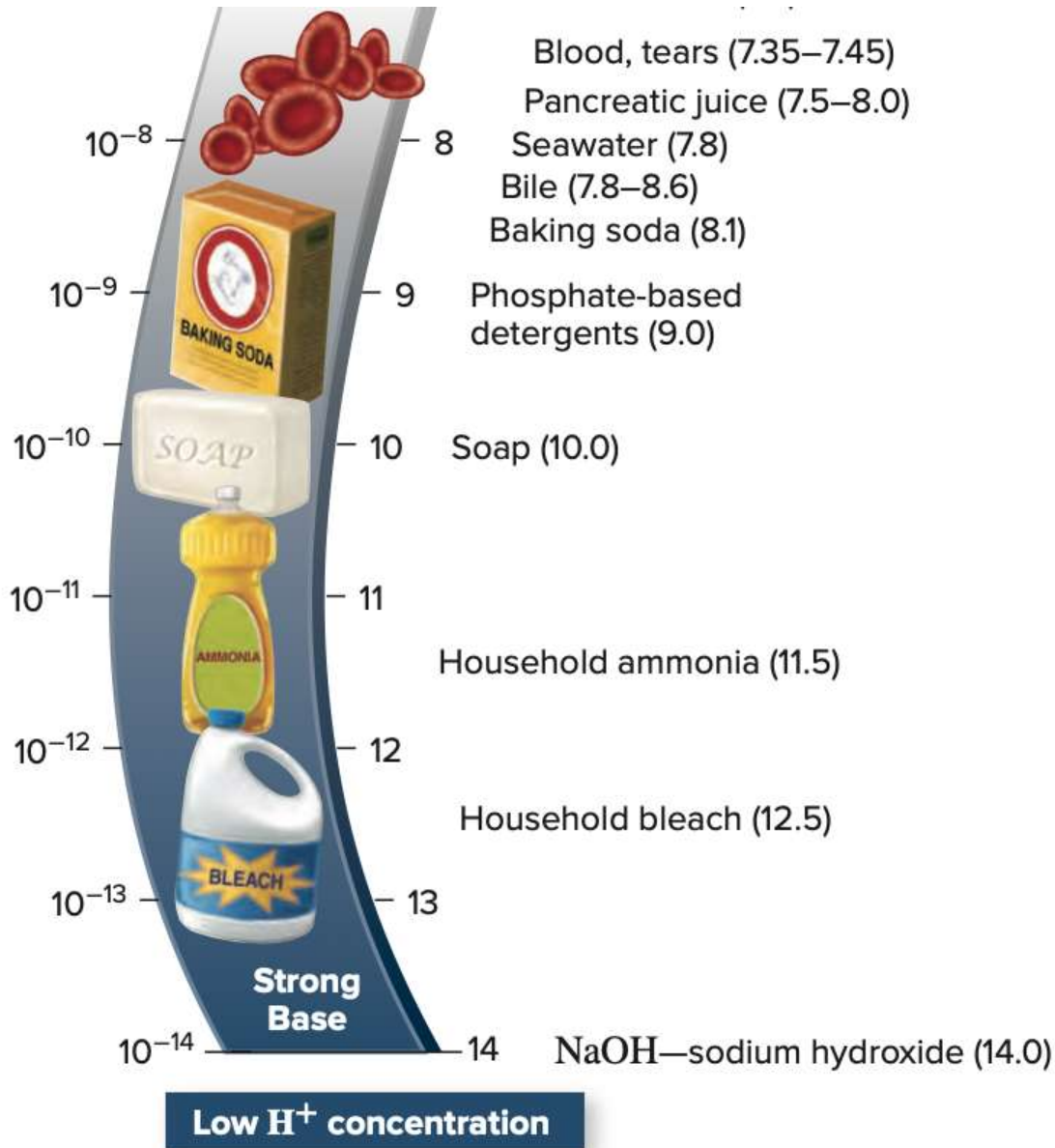
Acidic solution:

$$0 < \text{pH} < 7$$

An acid molecule
generate H^+ ions, like HCl



pH Scale



Basic solution:

$$7 < \text{pH} < 14$$

A basic molecule
generate OH⁻ ions, like
NaOH



pH Scale

Neutral solution: $\text{pH} = 7$

Pure water is neutral

$$[\text{H}^+] = [\text{OH}^-]$$

pH Scale

Neutral solution:

$$\text{pH} = 7$$

Pure water is neutral

$$[\text{H}^+] = [\text{OH}^-]$$

OBSERVATIONS

✓ $[\text{H}^+] \times [\text{OH}^-]$ is always
equal to 10^{-14}

✓ **pH + pOH is always equal
to 14**



Chemistry of Life

Pt. 2

Prof. Dr. Chiara Valsecchi

Course Goals

- Understand what are functional groups
- Understand basic concepts about the Building Block of Biomolecules
- Learn characteristics to distinguish protein, lipids and sugars

Carbon Based Molecules

Organic means “to contain carbon” and “to come from living things”.

Compounds that are organic contain carbon atoms that are covalently bonded together with other carbon atoms as well as other elements.

Carbon atoms that bond with each other and hydrogen atoms are called **hydrocarbons**.

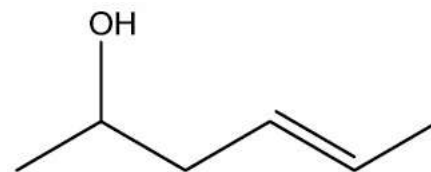
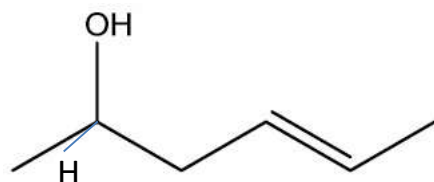
Functional Groups

ORGANIC MOLECULE :

The core structure (**backbone**) is made by **apolar** covalent bonds, and can form long chains.

However, to determine different functionality for each molecule, we have specific groups of atoms (with O, N, P, S) called **functional groups**

All of this is possible because Carbon can make up to 4 covalent bonds



Functional Groups

Most important in:

Name	Structure	Formula
Hydroxyl group	—O—H	—OH
Carboxyl group	$\begin{array}{c} \text{O} \\ \parallel \\ \text{—C} \\ \diagdown \\ \text{O—H} \end{array}$	—COOH
Amino group	$\begin{array}{c} \text{H} \\ \diagup \\ \text{—N} \\ \diagdown \\ \text{H} \end{array}$	—NH_2
Phosphate group	$\begin{array}{c} \text{O} \\ \parallel \\ \text{—O—P—O}^- \\ \\ \text{O}^- \end{array}$	—PO_4^{-2}

Carbohydrates

Lipids/protein

Protein

Nucleotides



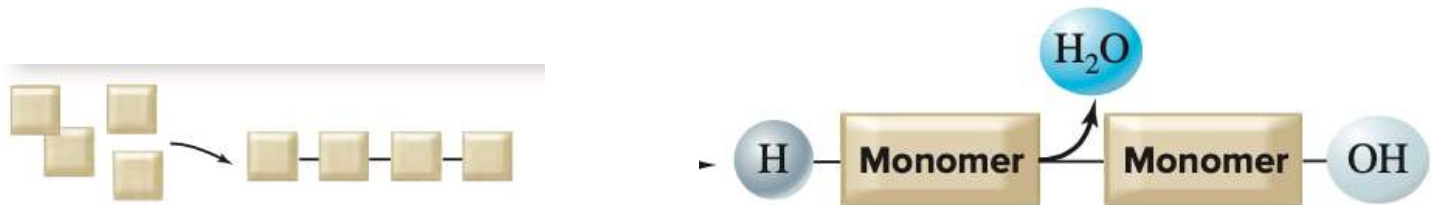
These 4 families of molecules constitute the building block of life!

Polymers

Carbohydrates, Lipids, Protein, Nucleotide are all POLYMERS:

Smaller units make up for long and large molecules.

The reaction to form polymers involves the **elimination of water**, so it is called DESHYDRATION.



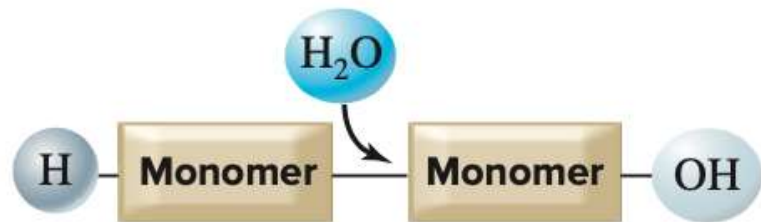
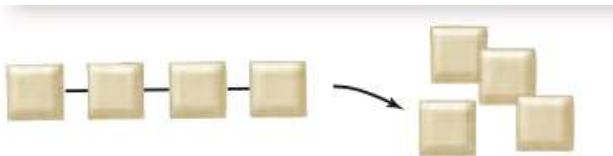
Polymers

Sugars, Lipids, Protein, Nucleotide are all POLYMERS:

Smaller units make up for long and large molecules.

The reaction to form polymers involves the elimination of water, so it is called DESHYDRATION.

The reaction to break down polymers needs **addition of water**, so it is called HYDROLYSIS.



Biological Polymers

1. Carbohydrates
2. Proteins
3. Lipids
4. Nucleotides

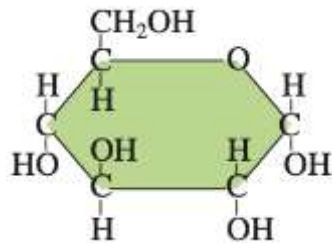
Any biological important molecule inside the cell can be classified into one of these 4 groups of organic molecules.

1. Carbohydrates

SUGARS

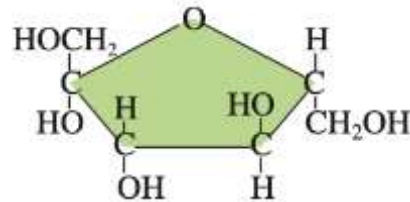
Monosaccharide

Dissacharide



Glucose

Energy for the
brain



Fructose

Important in
cellular
respiration

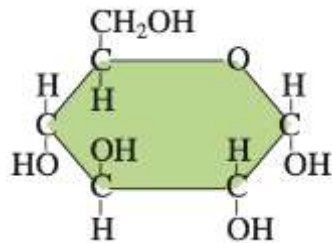
1. Carbohydrates

SUGARS

POLYSACCHARIDES

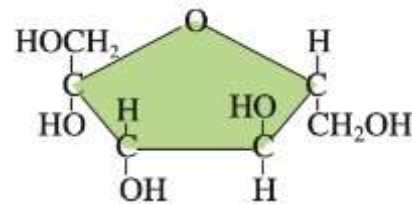
Monosaccharide

Dissacharide



Glucose

Energy for the
brain

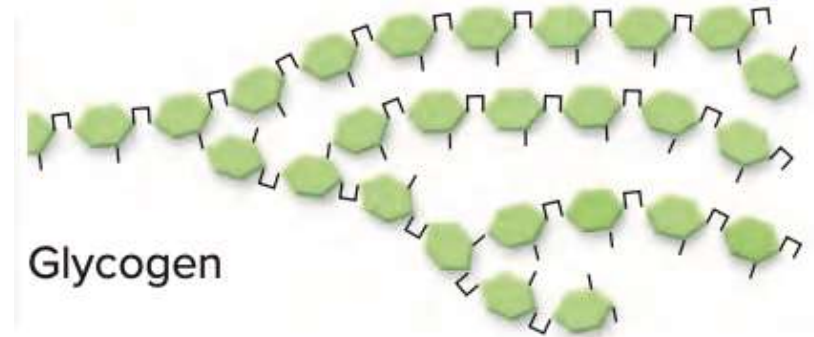


Fructose

Important in
celular
respiration



Cellulose



Glycogen

1. Carbohydrates

SUGARS

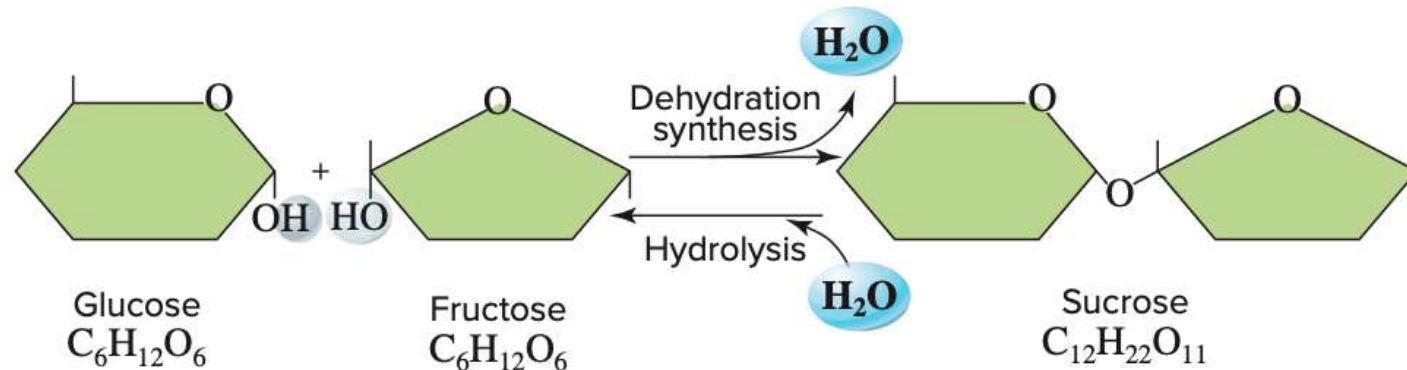
Monosaccharide

Dissacharide

POLYSACCHARIDES



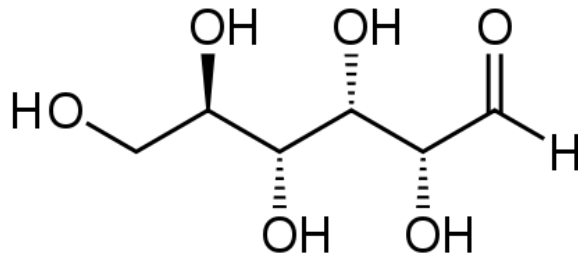
Cellulose



Common
sugar!

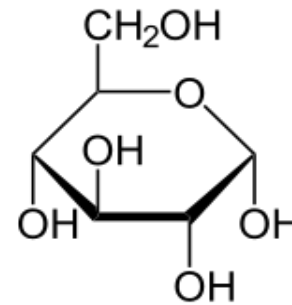
1. Carbohydrates

Monossacharides are rarely in the linear form, they tend to close up in a **cyclic structure**



Open structure

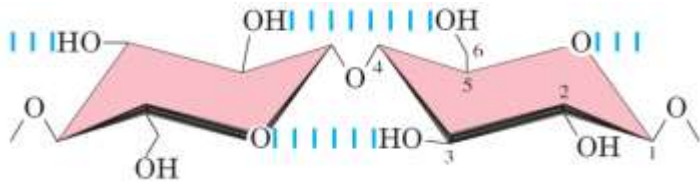
D-glucose



Closed structure

The reaction is called Glycoside formation

Cellulose



D-glucose $\beta(1 \rightarrow 4)$.

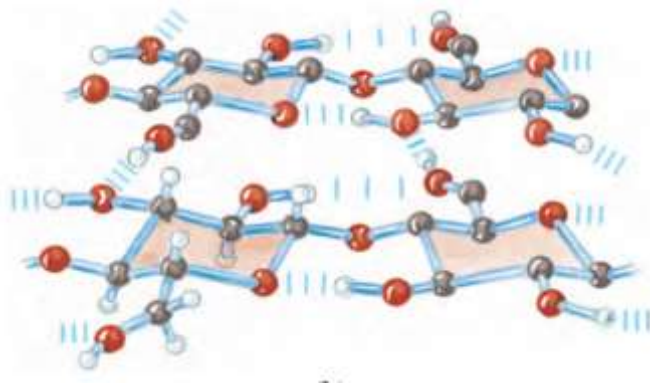
Linear, stabilized by hydrogen bond

Fibrous, resistant

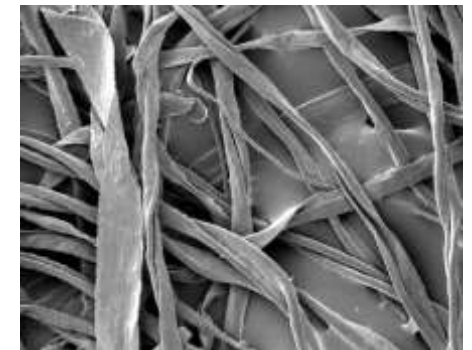
Insoluble in water

Plant cellular wall, wood structure,

Cotton is almost pure cellulose

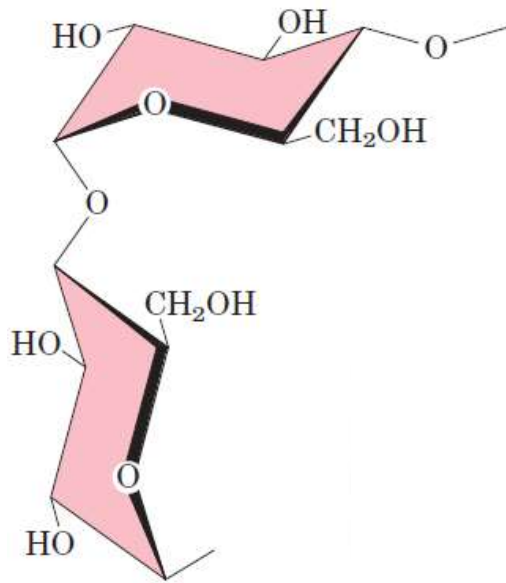


Cotton Fibers



Cotton Fibers

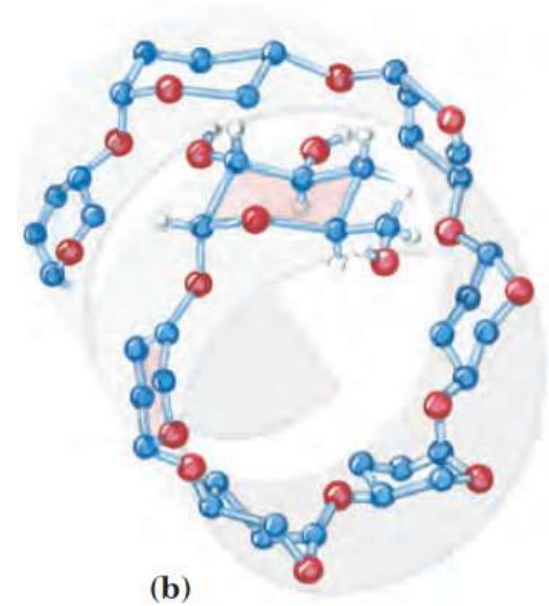
Starch



only GLUCOSE

The structure is folded
in a helix shape

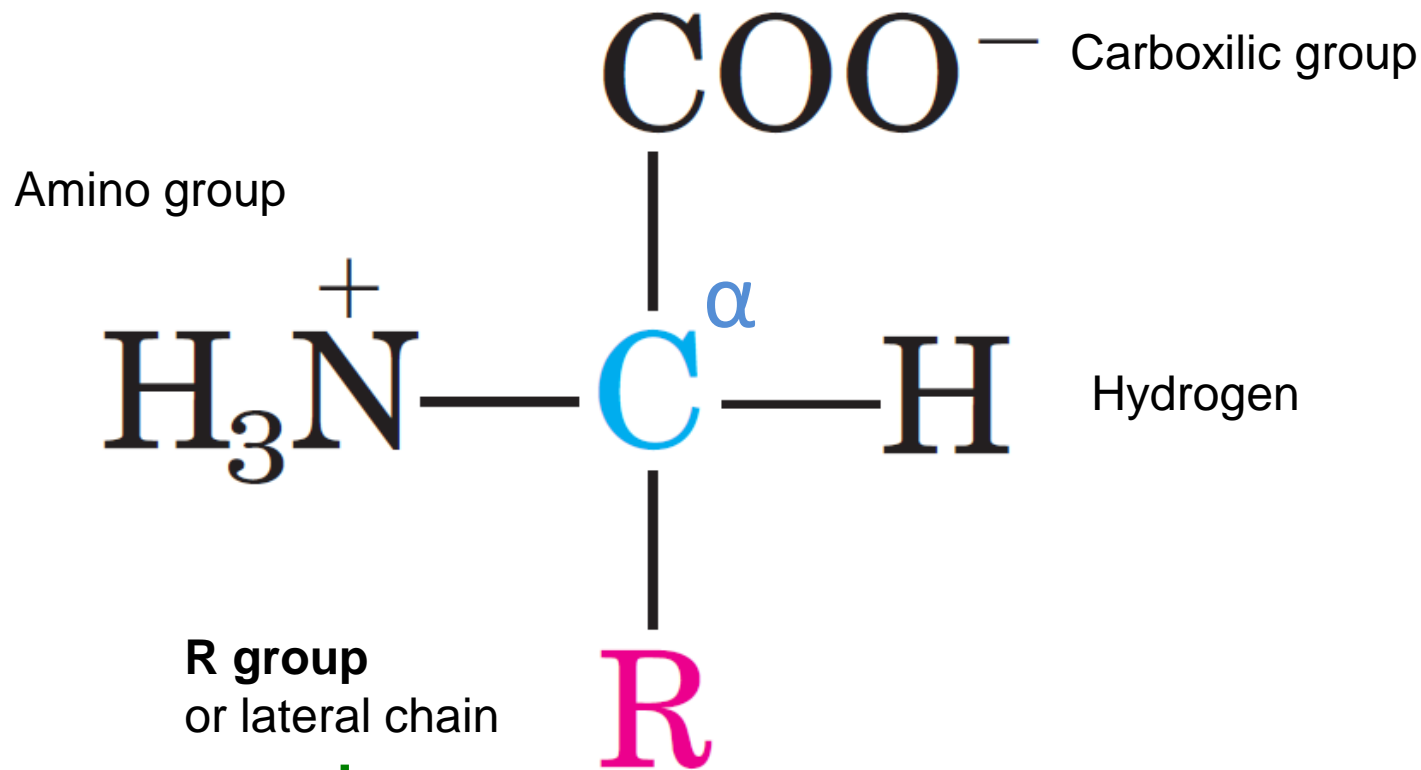
Energy storage for
living beings.



Starch in plants

GLYCOGEN in animals and fungi

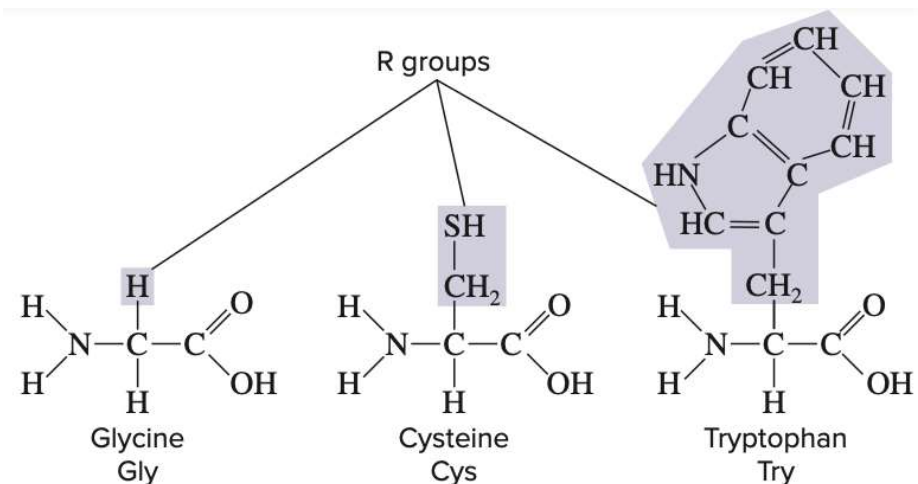
2. Proteins



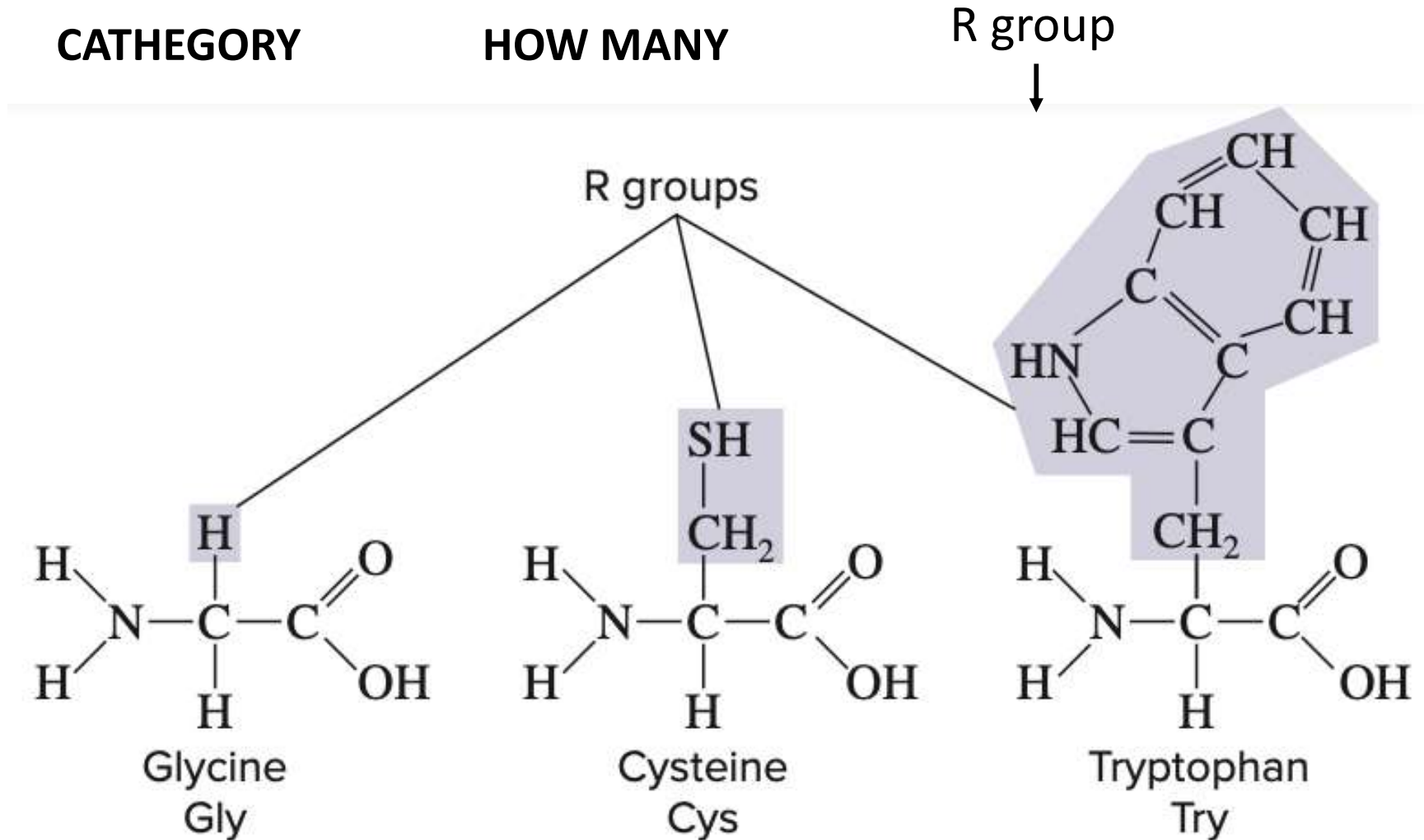
The R group defines aminoacid properties, as structure, size, charge and solubility

Aminoacid classification

CATHEGORY	HOW MANY	R group ↓
1. Apolar:	7	TOTAL: 20 different types Aminoacid = aa
2. Polar:	5	
3. Aromatic :	3	
4. Positively charged:	3	
5. Negatively charged:	2	



Aminoacid classification



Aminoacid Interactions Overview

Int. van der Waals:

Apolars

Dissulfite bond:

Cystine

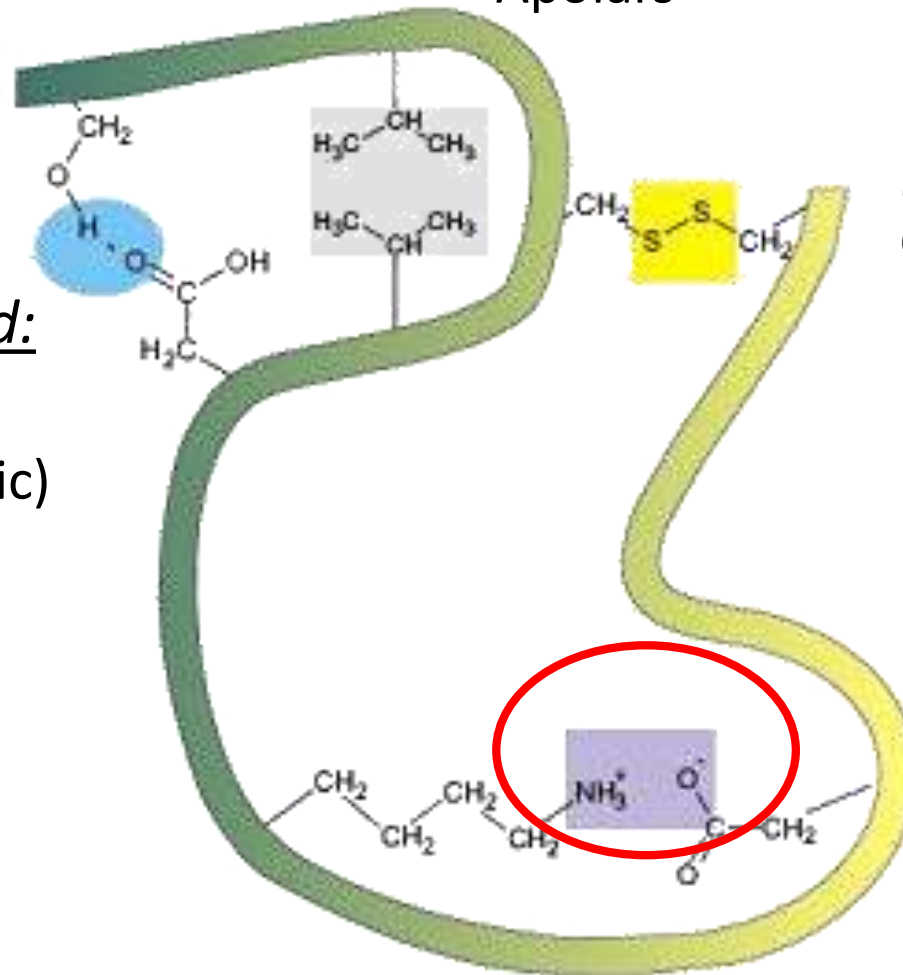
Hydrogen Bond:

Polars

Tyrosin (aromatic)

Ionic Bond:

Charged
aminoacids



2. Proteins

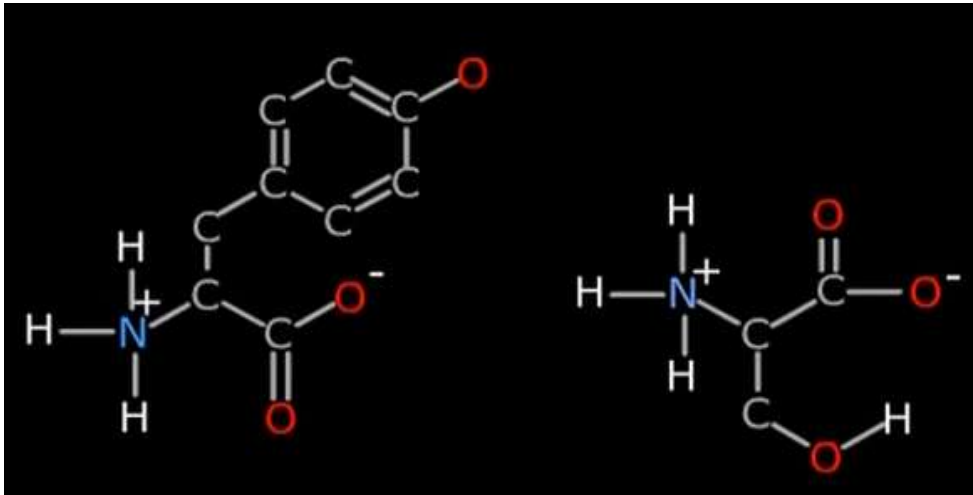
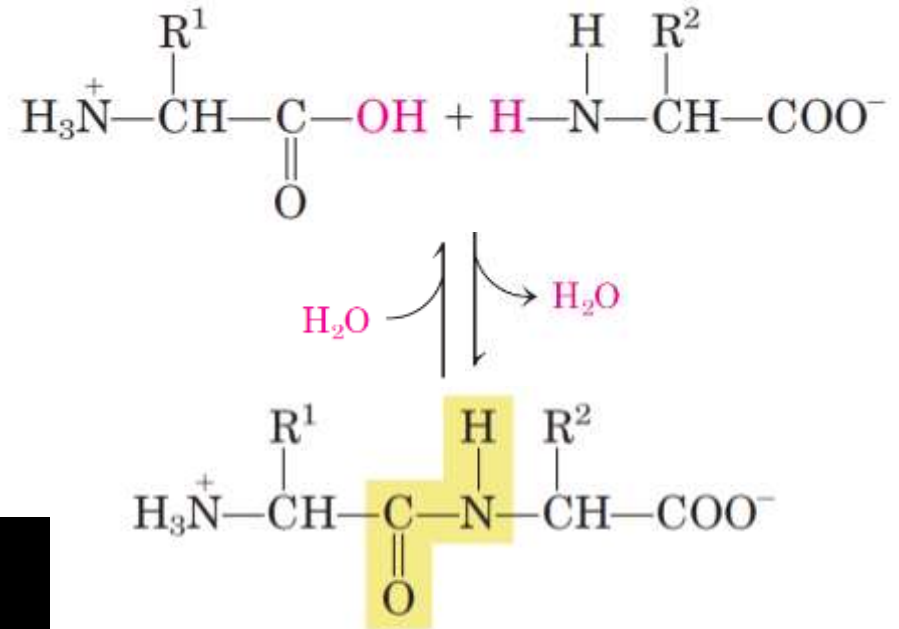
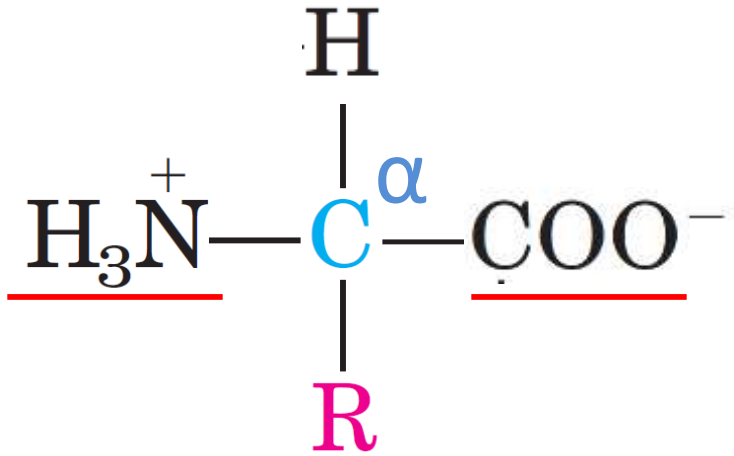
Peptides: less than 10 aa

Oligopeptides ($10 < \text{aa} < 100$) and Polypeptides (> 100 aa)

Proteins are the functional core of the cell: antibodies, enzymes, receptors and cell skeleton.

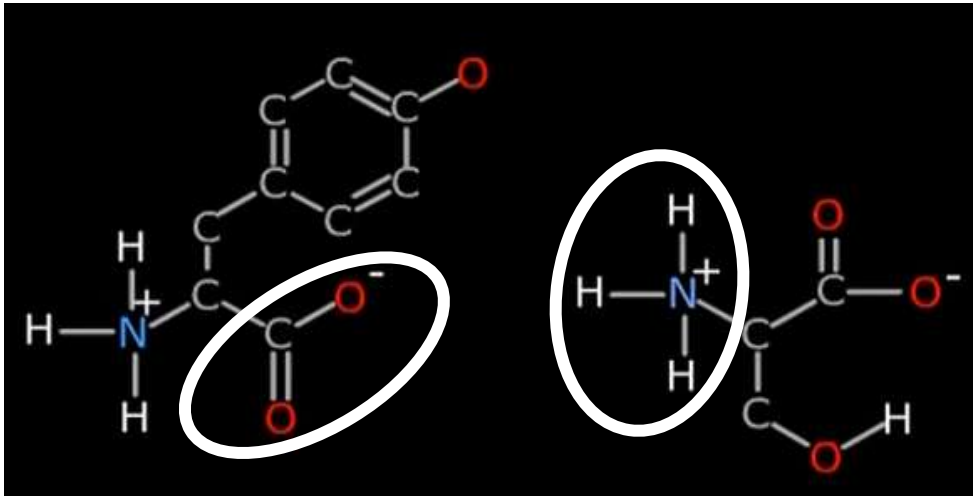
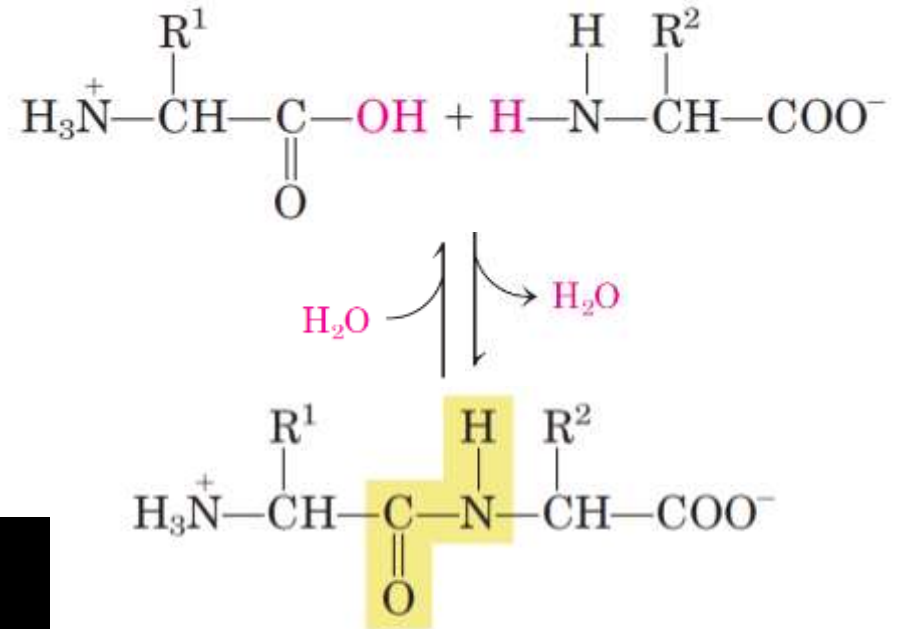
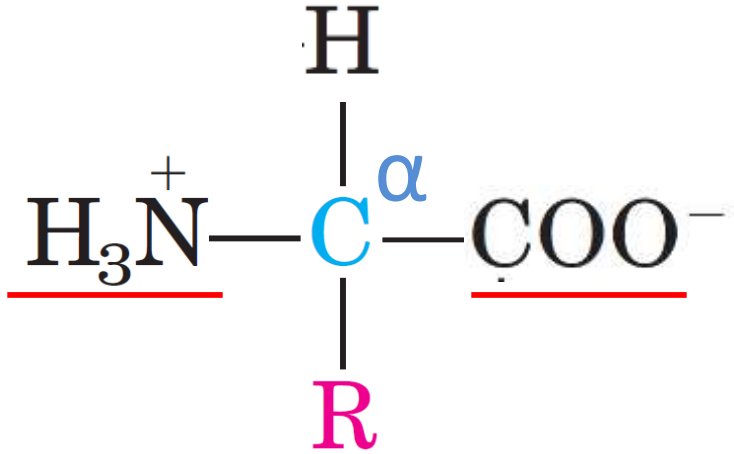
The **function depends on their structure**, so it is extremely important

Protein Formation



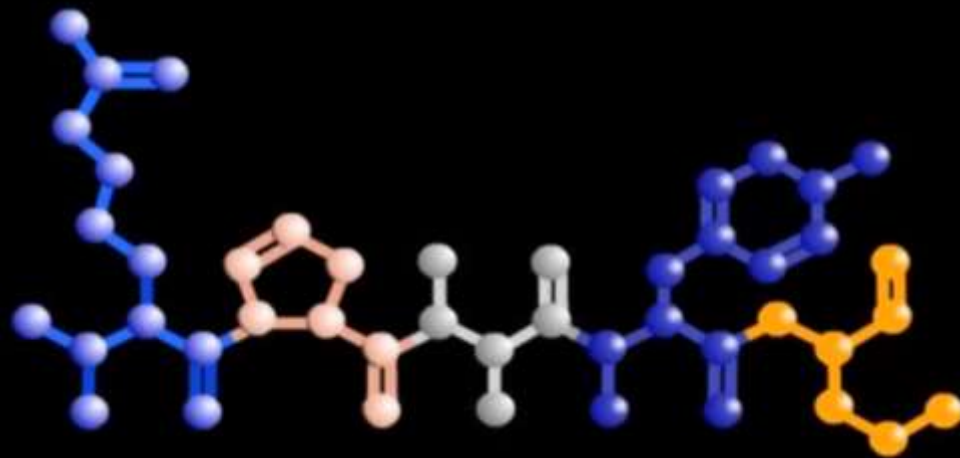
Condensation / Hydrolysis

Protein Formation

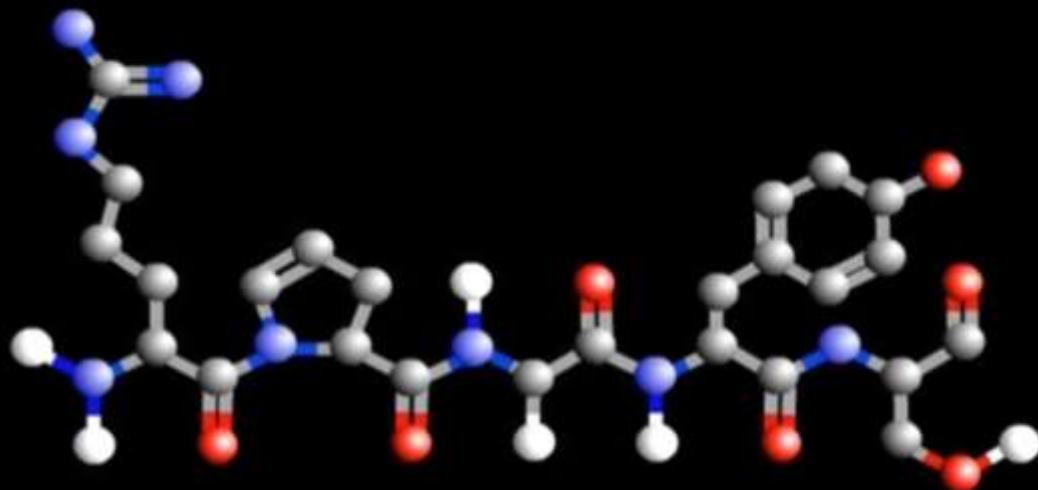


Condensation / Hydrolysis

2. Proteins

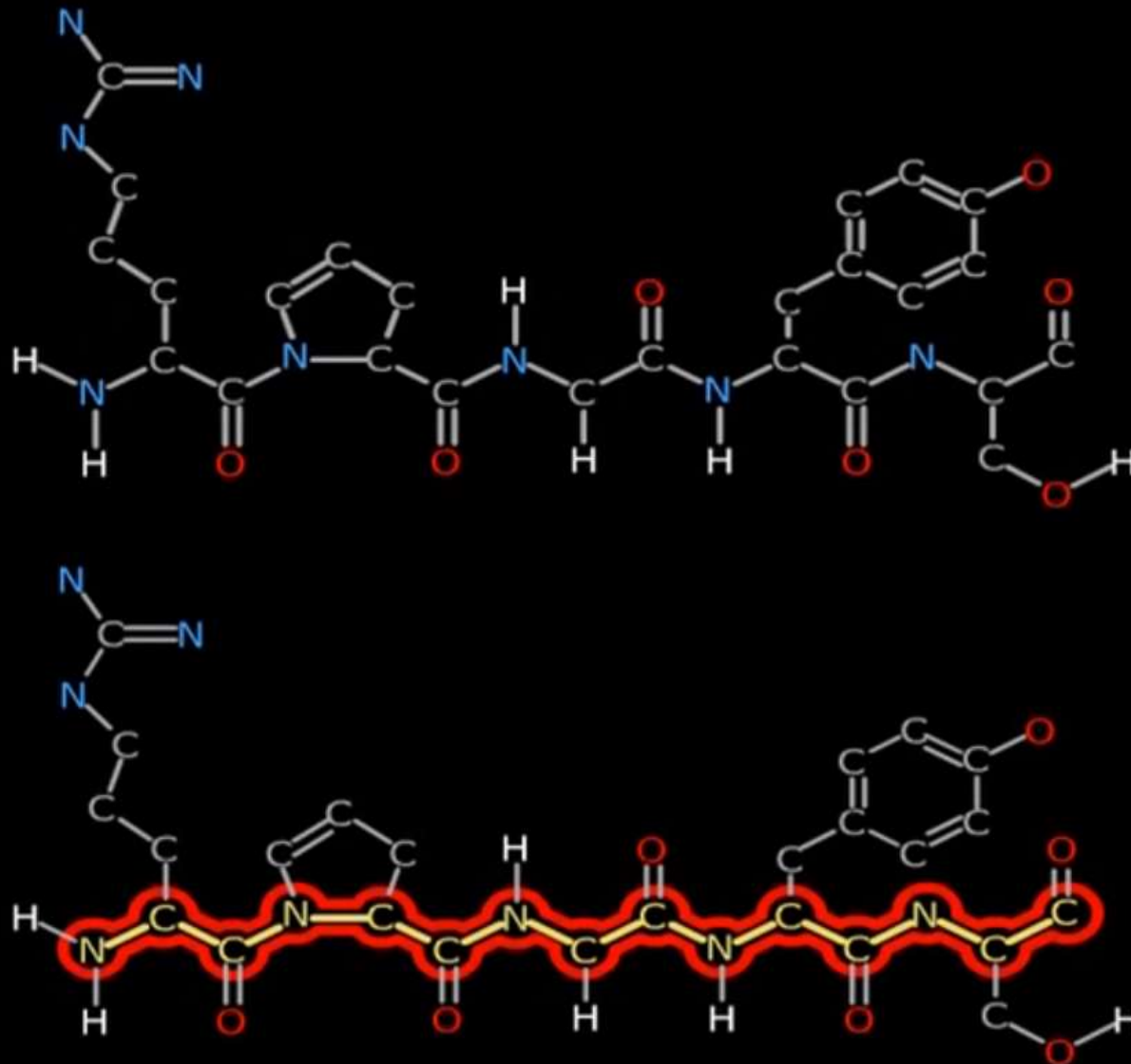


Peptide: 5 aminoacids



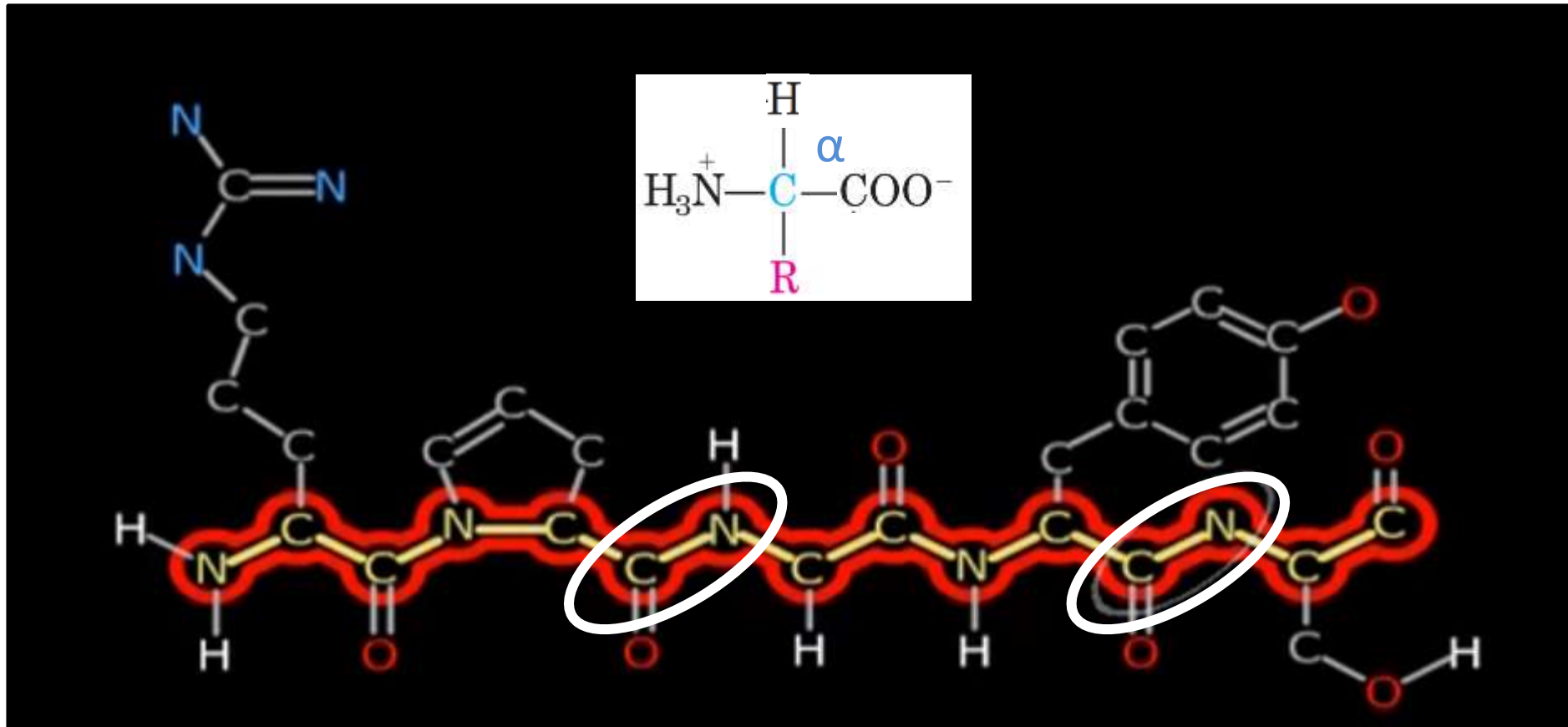
Atomic model, without H

Ligação Peptídica



Protein backbone

Primary Structure



Primary Structure: the linear sequence of aminoacid

Secondary Structure

Secondary Structure: spatial arrangement of close aminoacid, which create well-defined 3D structures.

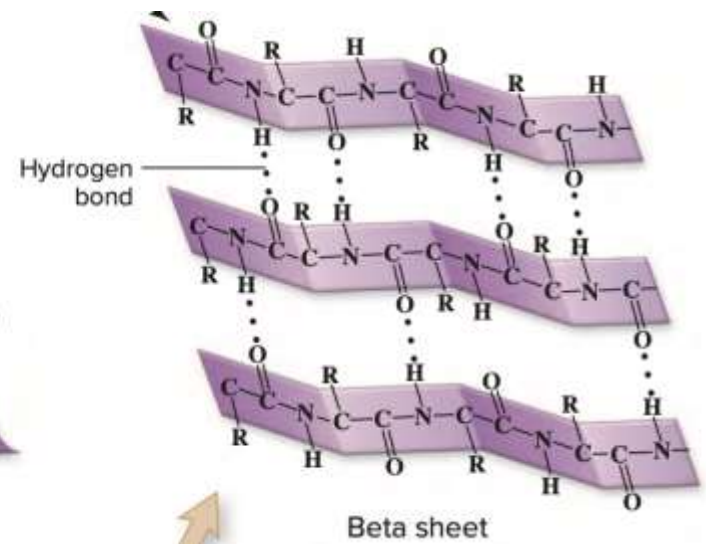
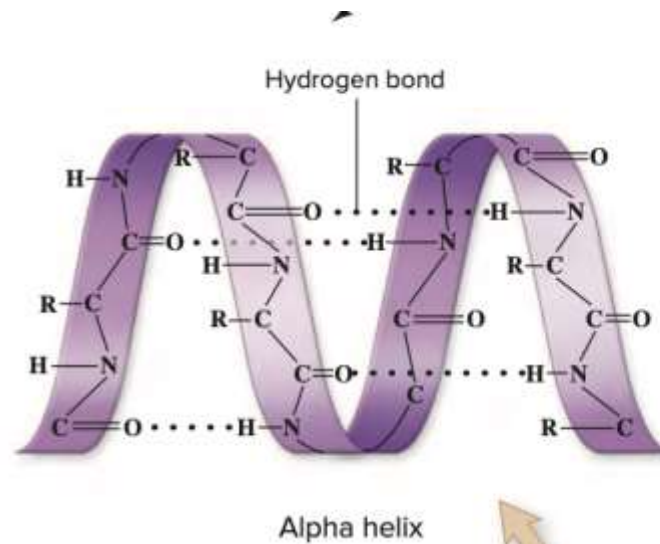
Types:

α Helix

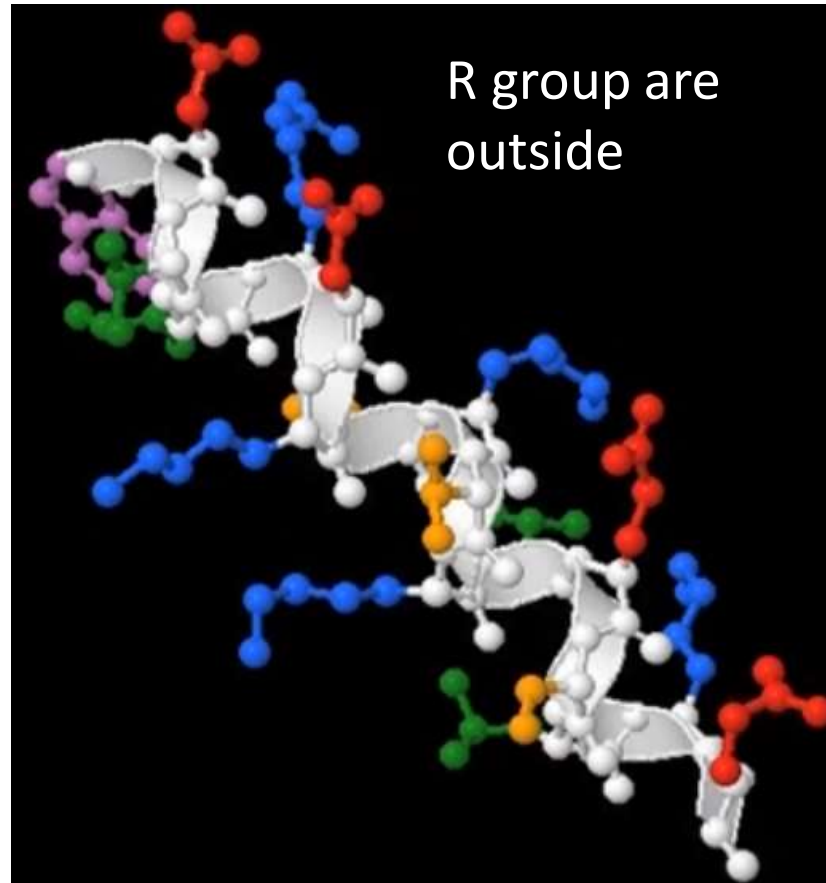
β sheets

Coils

Turns



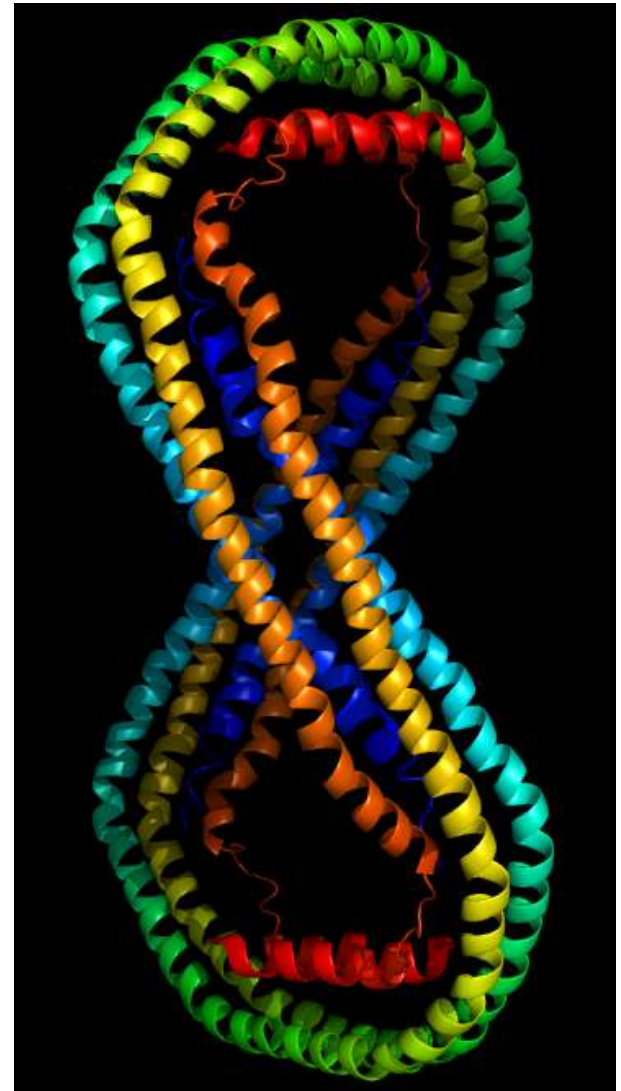
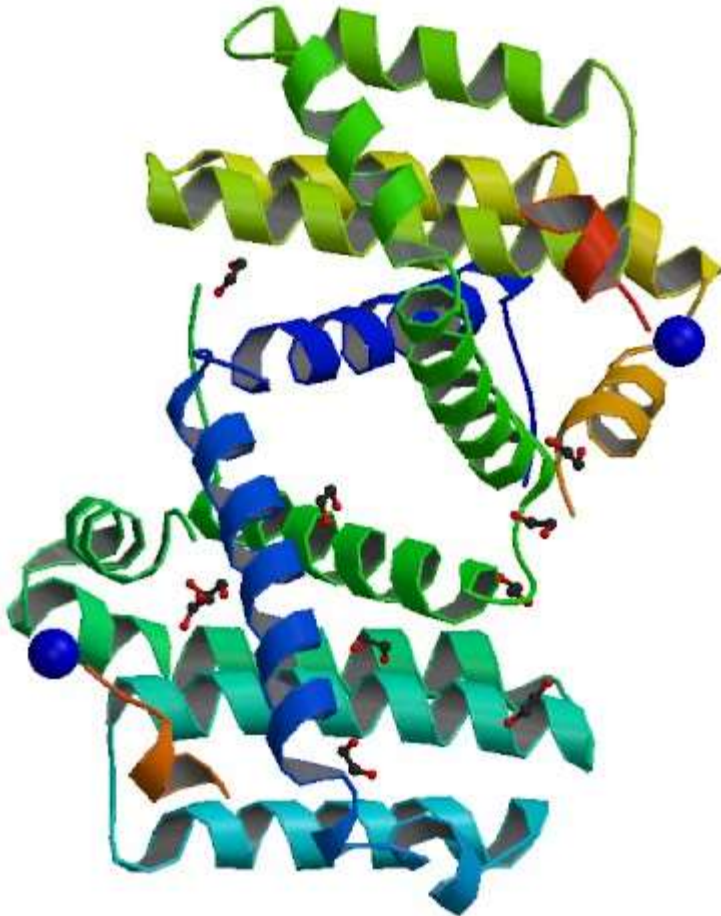
α - helix



IMPORTANT! Is the primary structure that determine the correct sequence for these structure to happen!

α – helix protein

apolipoprotein A-I (PDB code 1AV1)



β sheets



The interaction is between atoms that can be far apart in the primary structure

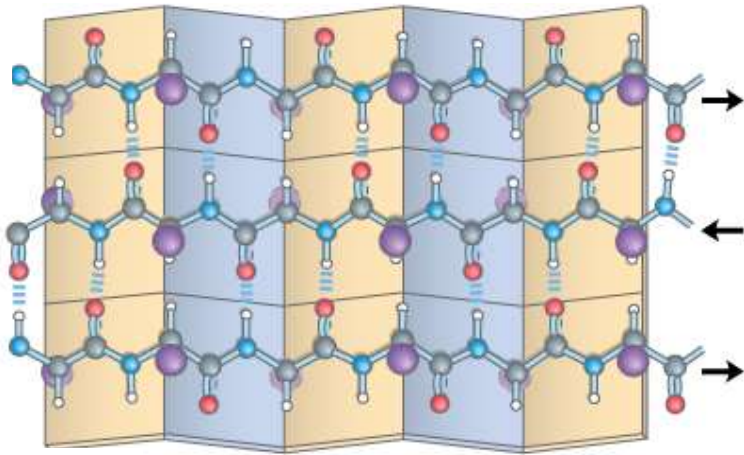
β sheets

R groups are above and below the sheet plane

The sequence is like a zig-zag due to hydrogen bonds

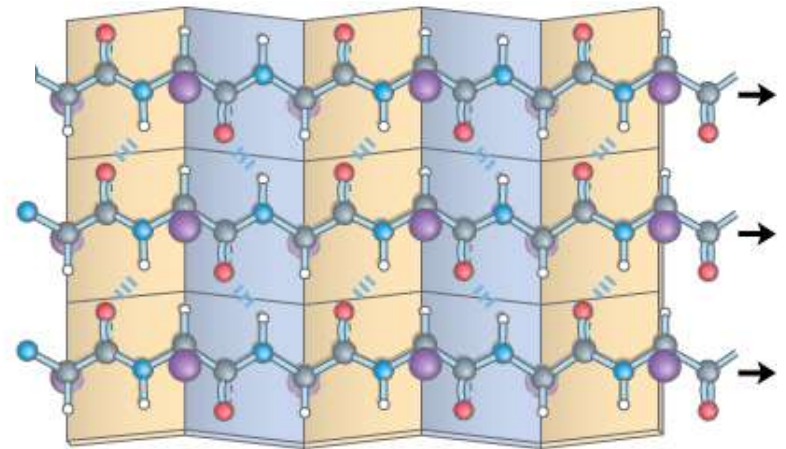
ANTIPARALLEL

Top
view

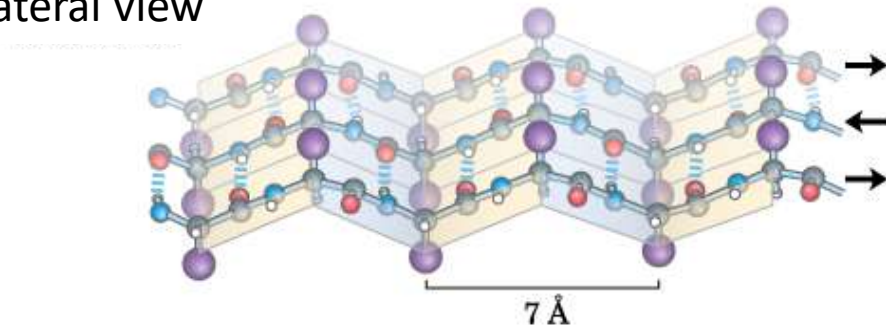


PARALLEL

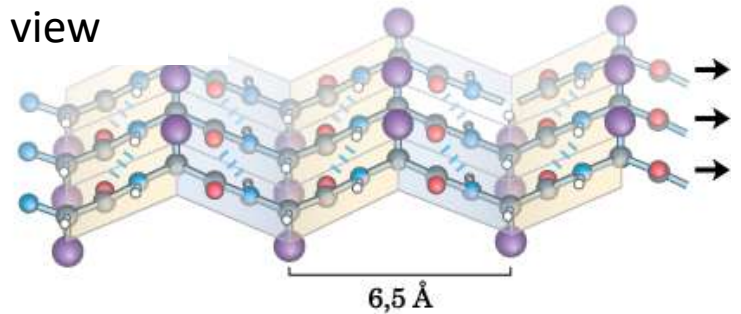
Top
view



Lateral
view

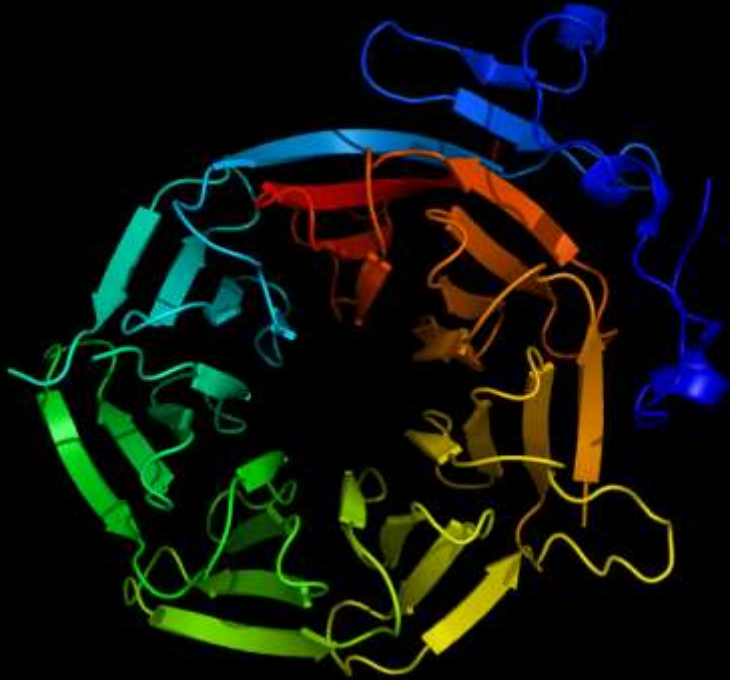


Lateral
view

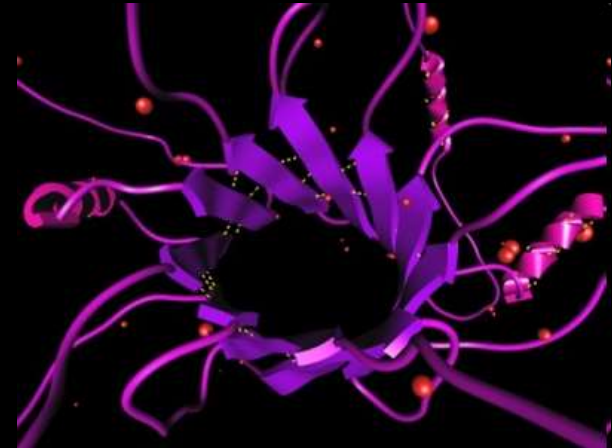


β sheets protein

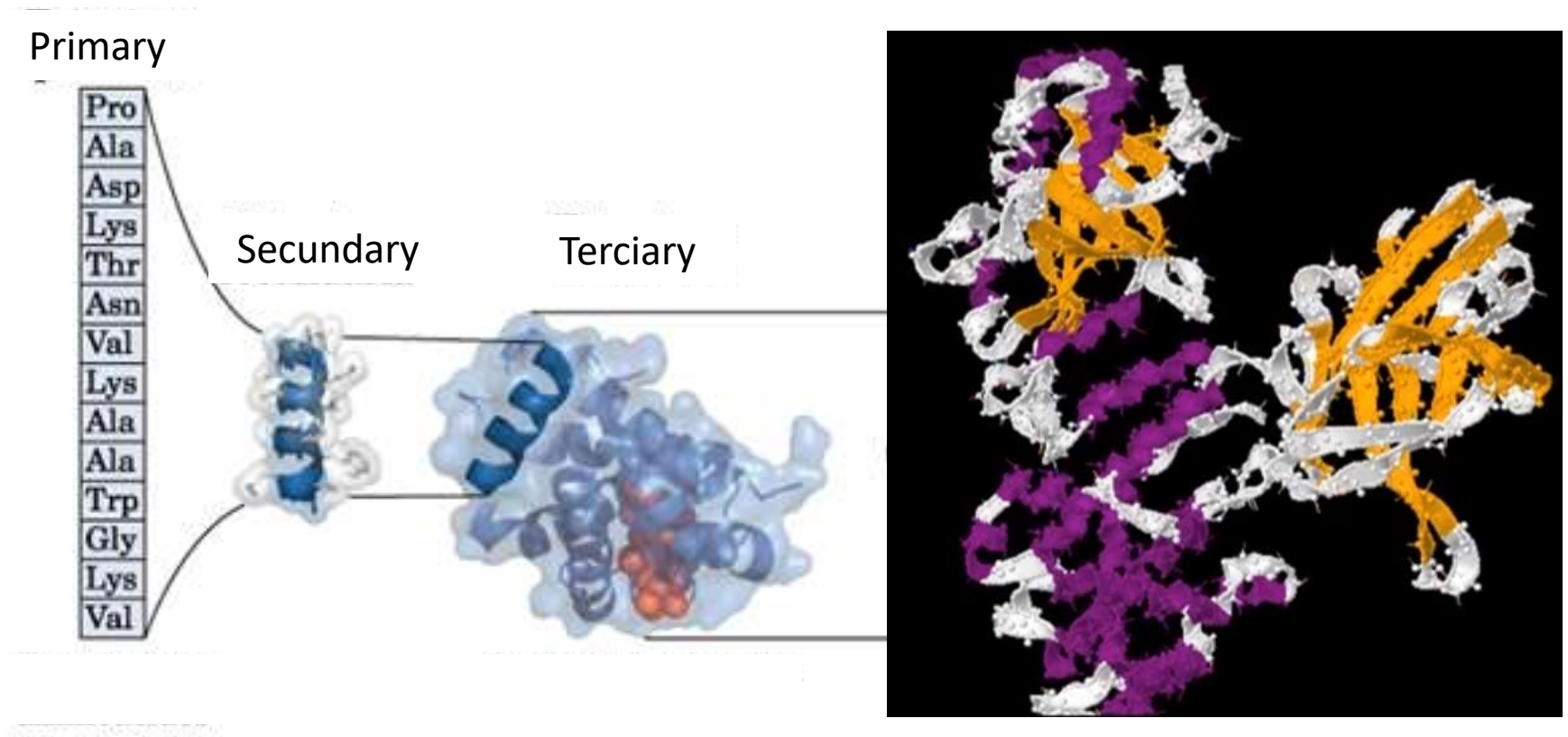
Beta-prupolsor



Beta-barrel

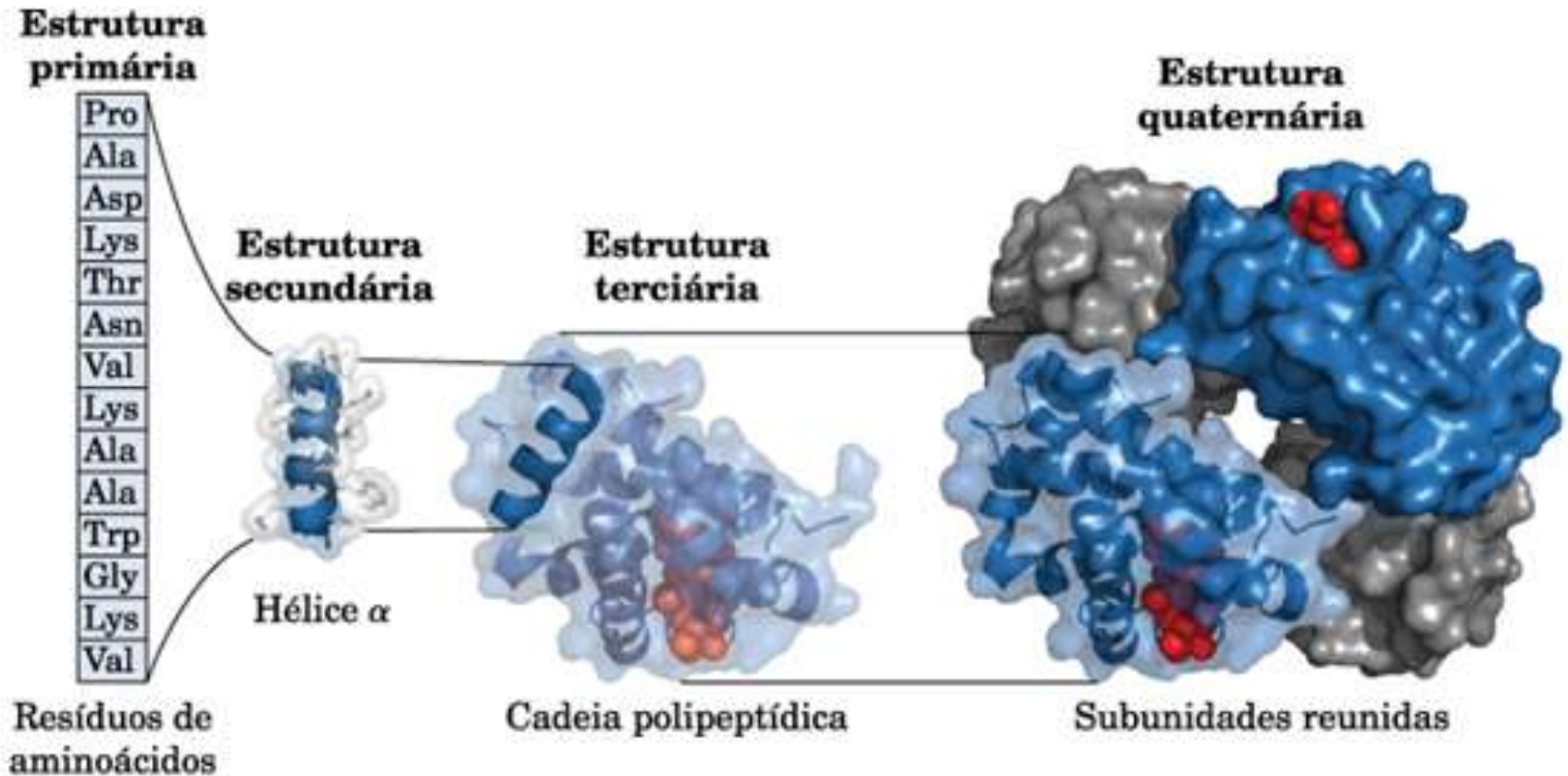


Tertiary Structure



Tertiary Structure: how the protein fold in space after the formation of the secondary structure patterns.

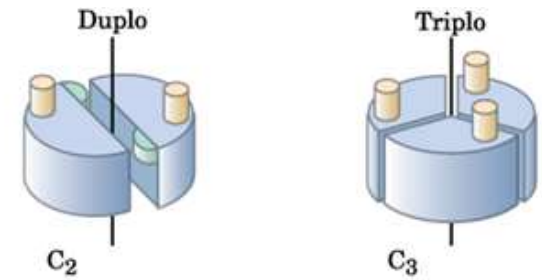
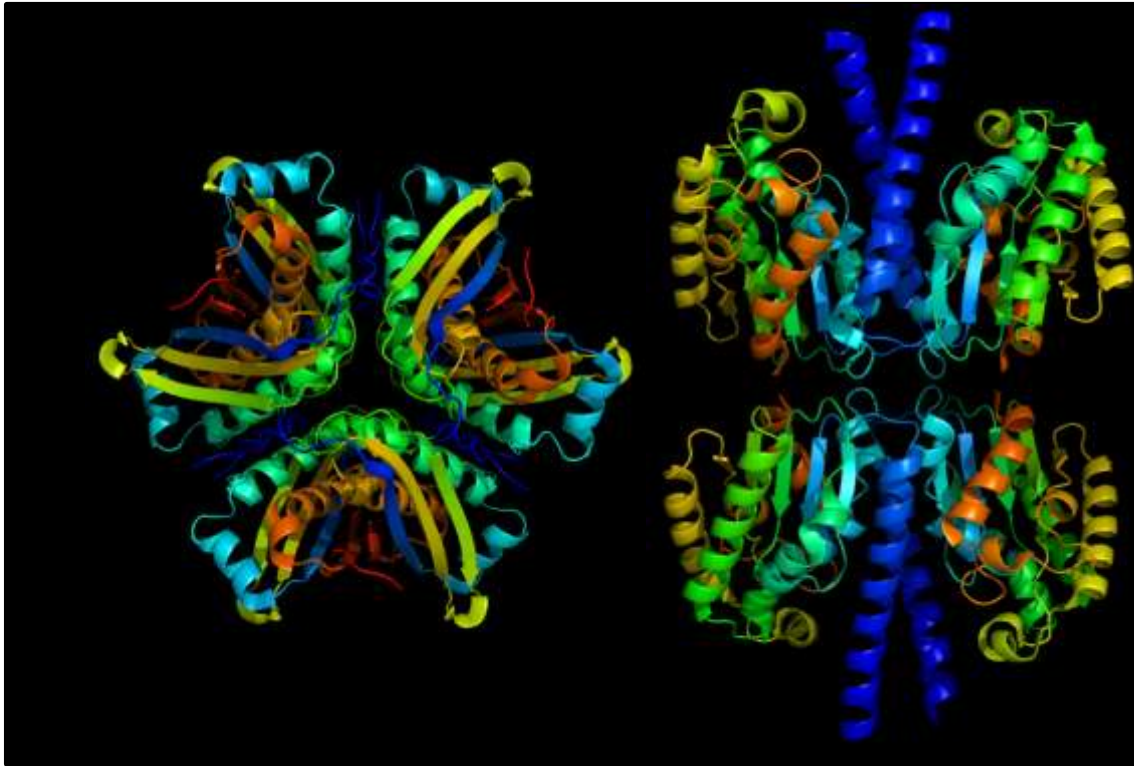
Quaternary Structure



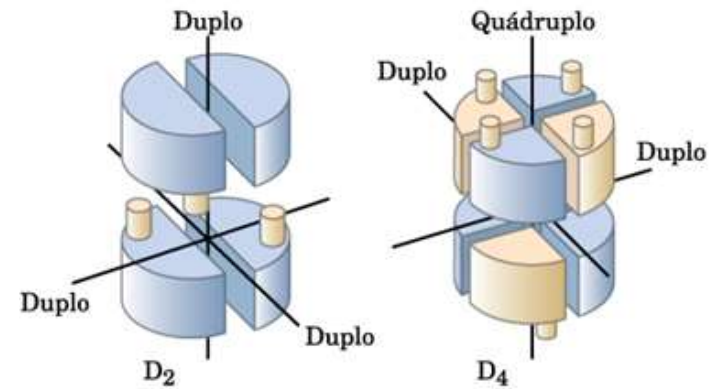
Quaternary Structure: different subunits of tertiary structures together to form complexes

Quaternary Structure

Dimers, Trimers, Oligomers



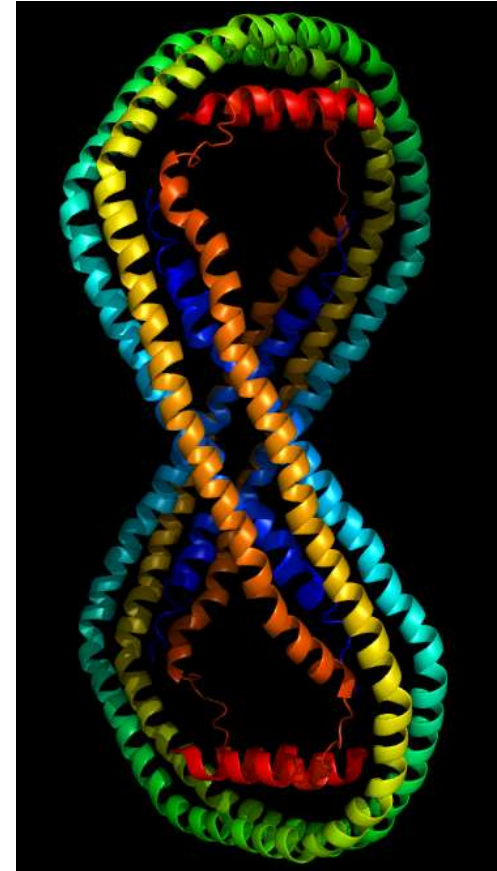
Dois tipos de simetria cíclica
(a)



Dois tipos de simetria diédrica
(b)

Important facts

1. The 3D conformation depends on the AA sequence
2. The main stabilizing forces are non covalente interactions
3. Common patterns (helix and sheets) help to stabilize
4. Protein always interact with water: hydration sphere
5. To function correctly, each protein has a specific structure, called NATIVE CONFORM

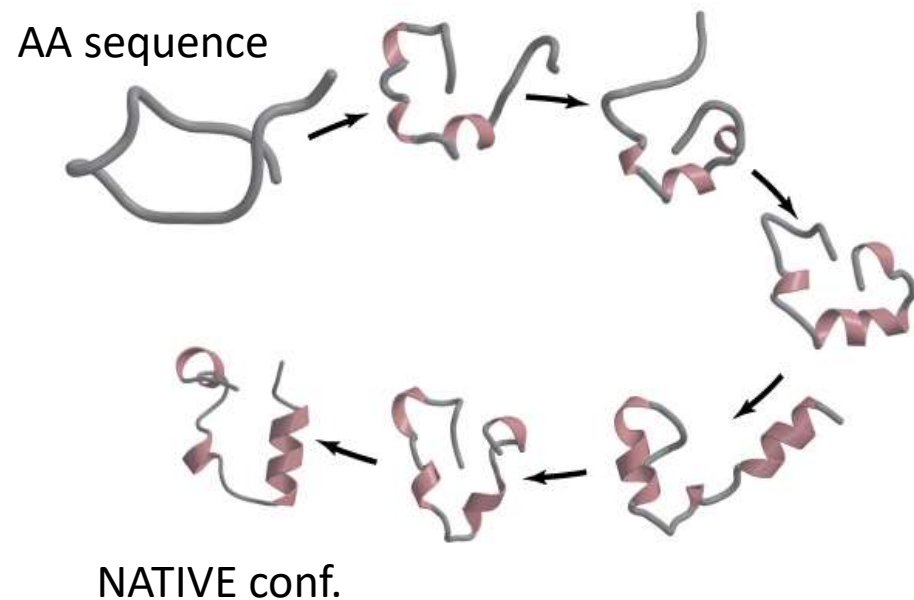


apolipoprotein A-I (PDB code 1AV1)
Estrutura formada apenas por alfas-hélices

Native Conformation

NATIVE CONFORMATION: the shape that gives the protein its function!

DESNATURATED CONFORMATION: part or all of the protein loses its folding: the function is also lost. Normally due to heat or Strong chemical attack.



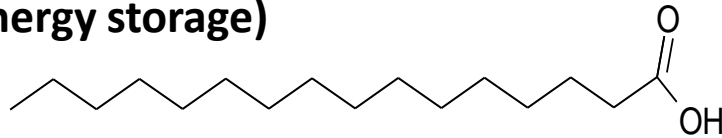
3. Lipids



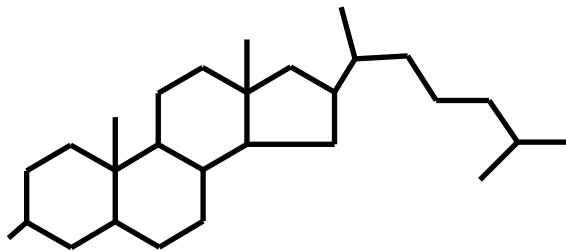
Biological Lipids

- It is a big group with many **different types** of molecules, depending on the function
- One common feature : **water insoluble**

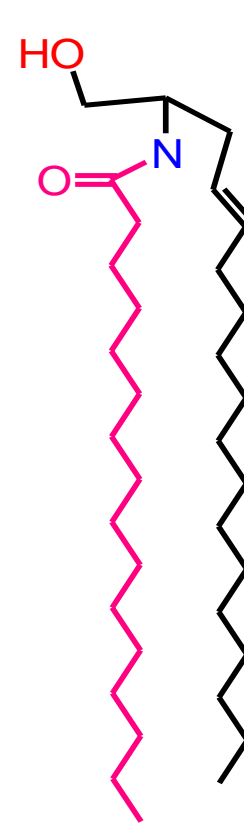
Fatty acid
(energy storage)



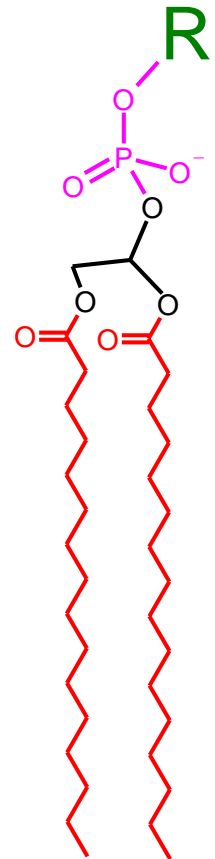
HO



Steroids (hormon)



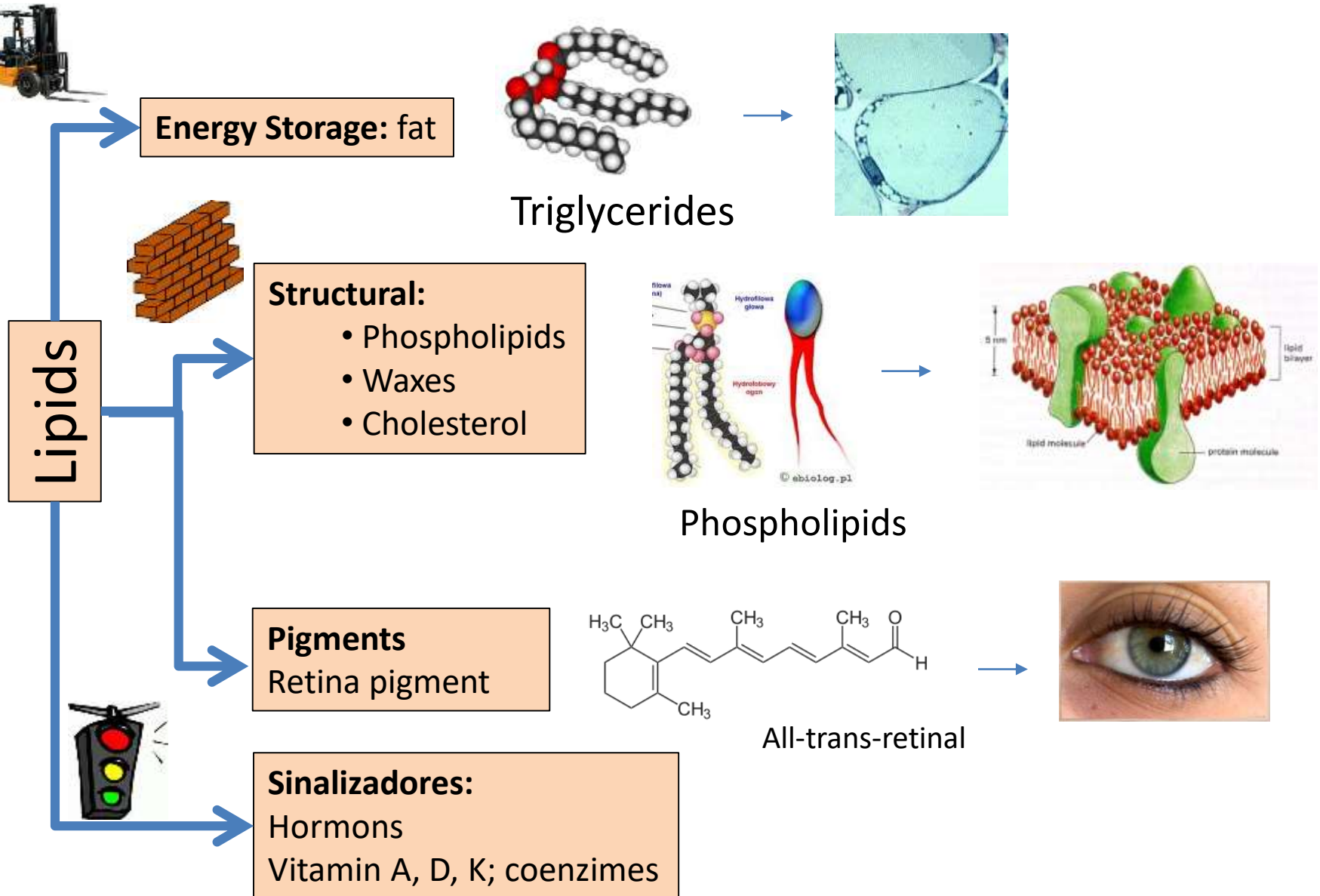
sphingolipid



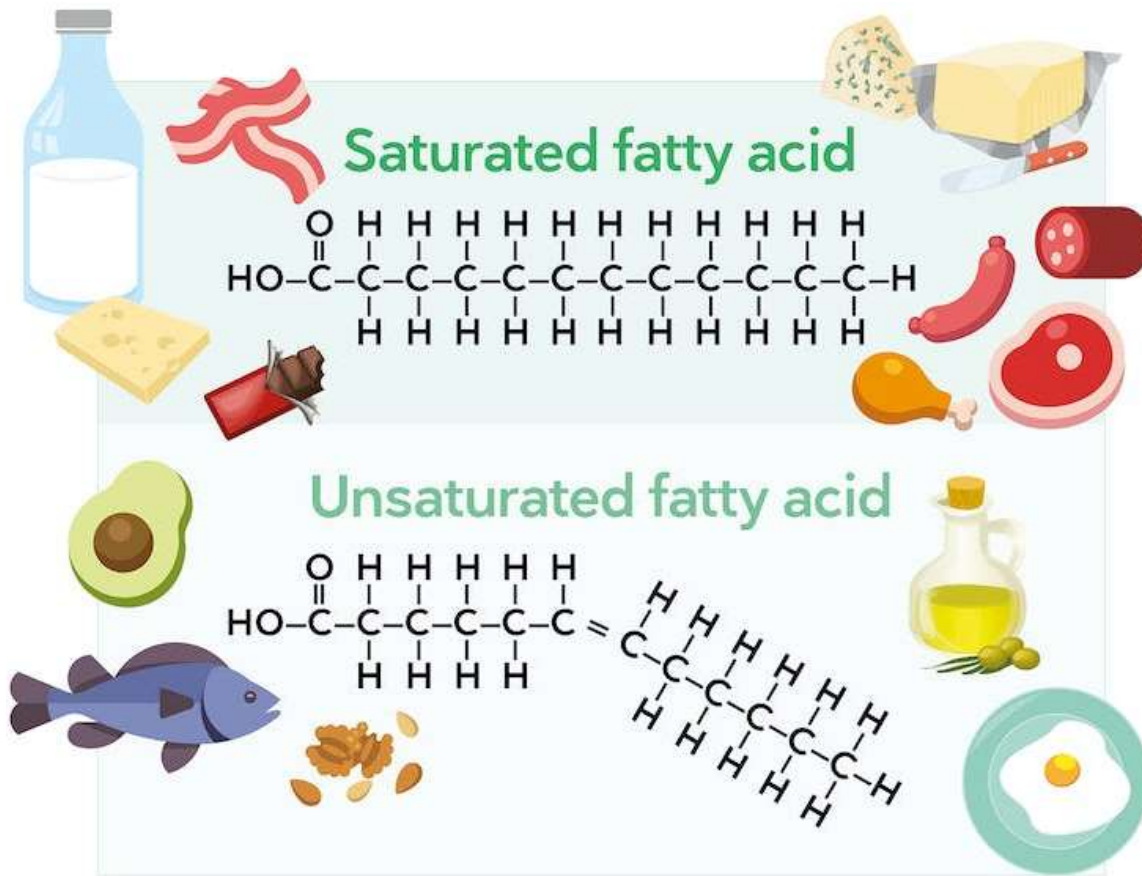
Phospholipid

Cell membranes

Lipid Functions



Saturated or Unsaturated



- **SATURATED:**

Each Carbon has the maximum number of Hydrogens (2).

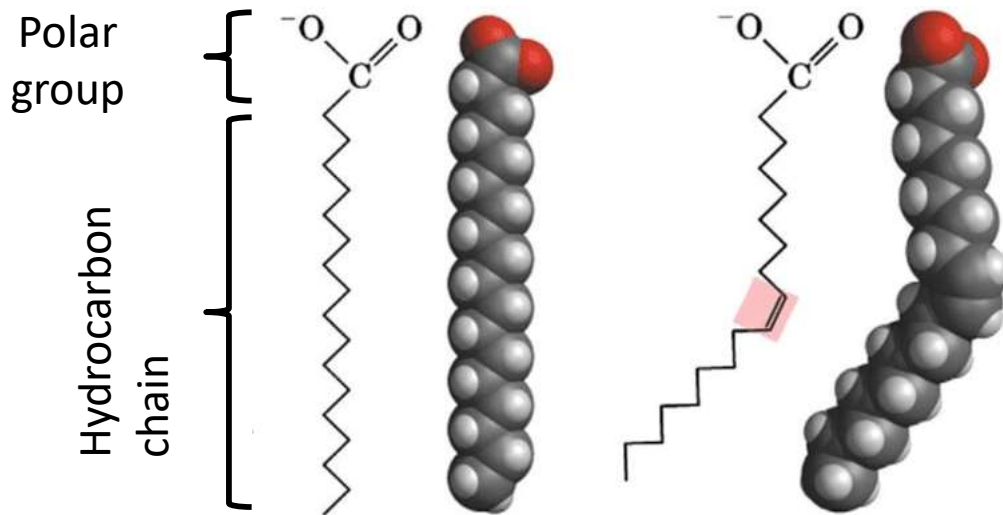
No healthy

- **UNSATURATED:**

Some carbons involved in double-bonds with other carbons, **less** Hydrogens.

Easy to break down, more healthy

Fatty Acids



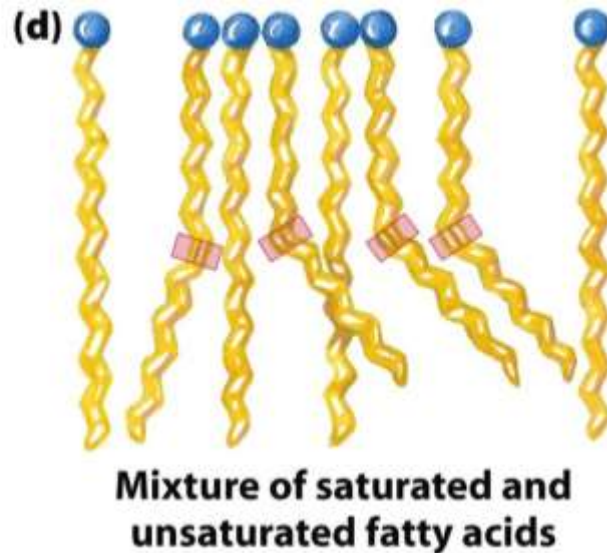
The saturation degree affects molecule stacking

The bend in unsaturated fatty acid causes more mobility and weaker interactions:



Less fusion temperature, so they are more soft or liquid at room temperature

Similar to wax



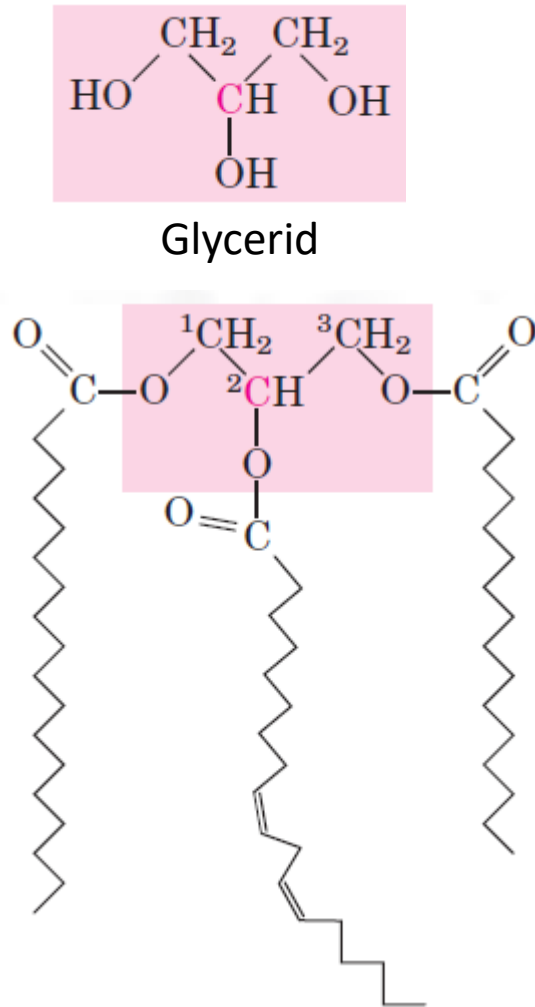
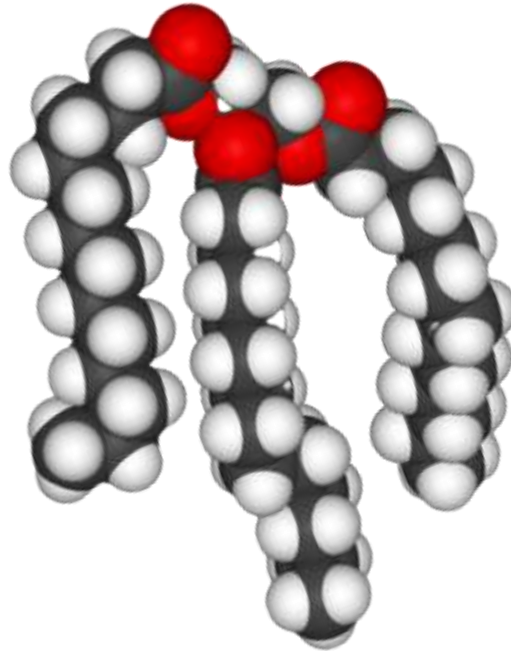
greasy liquid, oil

Triglycerids

Most important family of lipid for energy storage:

3 long fatty acid chain linked to a glycerol molecule.

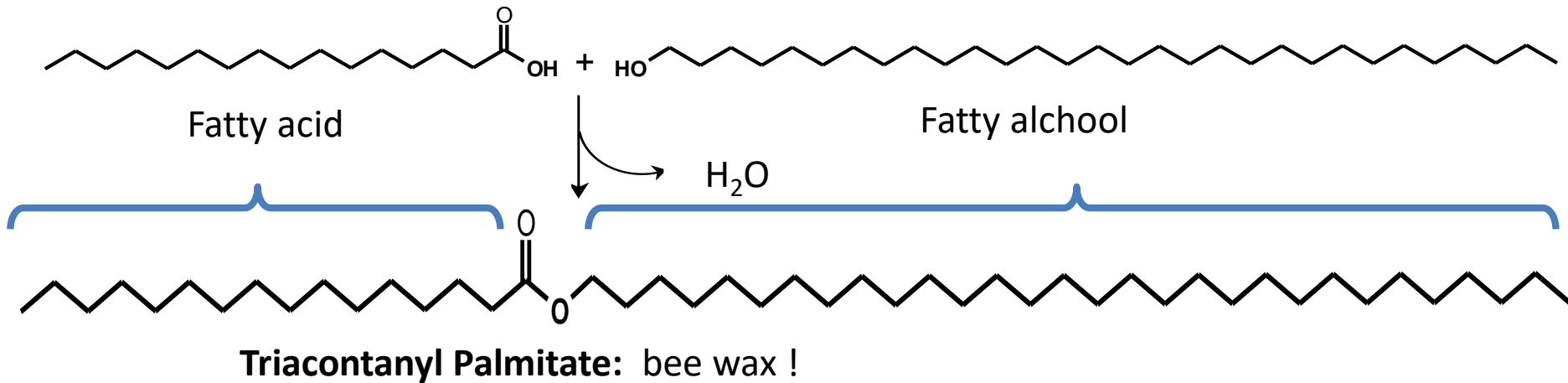
Stored in the adipocytes, the “fat” cells



1-Stearoyl , 2-linoleoyl, 3-palmitoyl
glycerol: a mixed triglycerid

Waxes

- Long fatty acid chains
- Highly water repellant



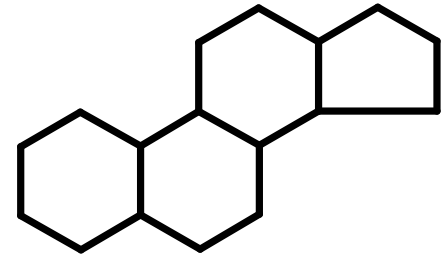
At 25°C the bee wax
is completely
waterproof



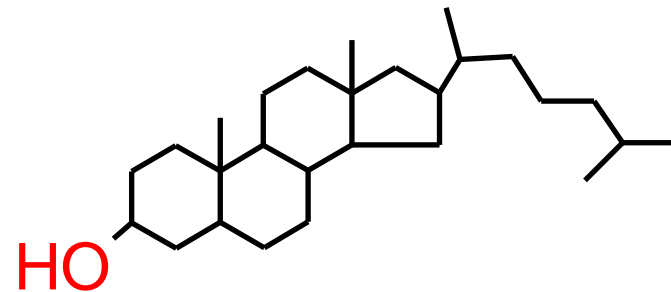
Wax color pencils

Steroid Family

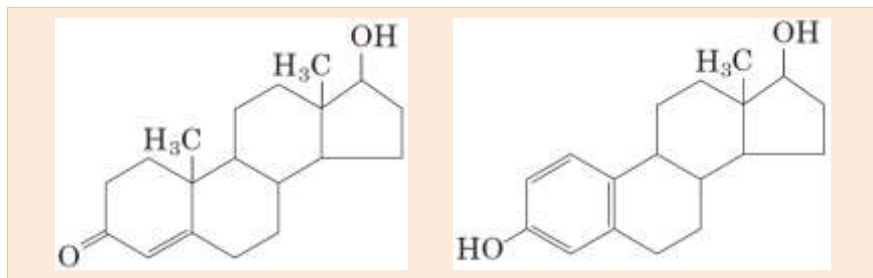
- Structural lipids present in most Eukaryotic membranes
- Core structure is rigid
- Cholesterol is the most important, however, it can be bad for health (good and bad cholesterol)
- Cholesterol is the base material for sex and anti-inflammatory hormones, vitamins (D) and biliar salts



Steroids core structure



Cholesterol



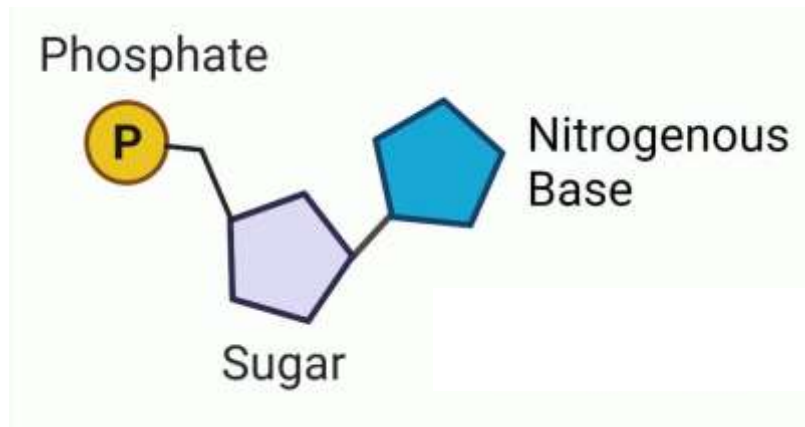
Testosterone

Estradiol

4. Nucleotides

Monomers that constitute the two nucleic acids: DNA (deoxyribonucleic acid) and RNA (ribonucleic acid).

The difference is in the sugar.

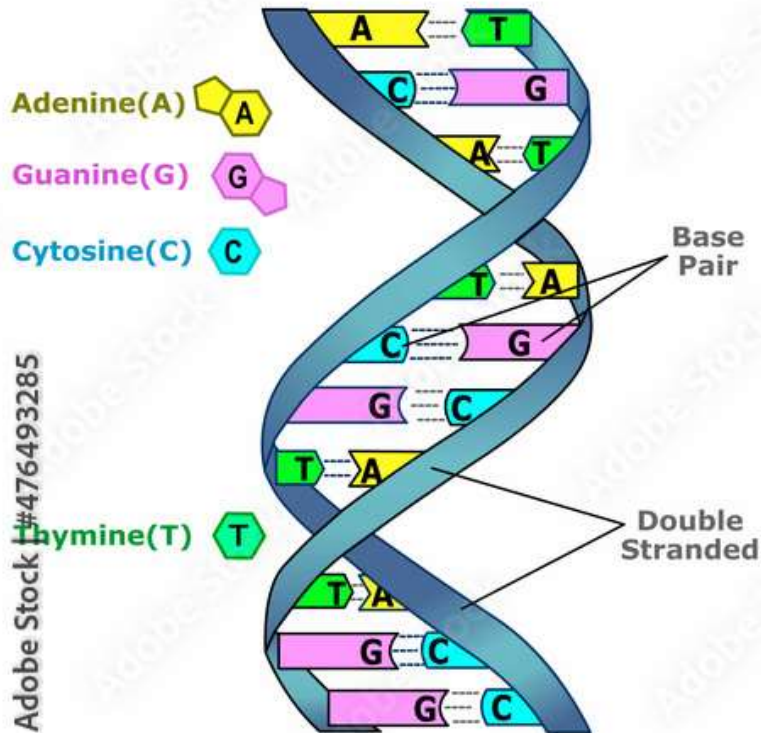


ADENINE
GUANINE
CYTOSINE
THYMINE
URACYL

Pairs: A-T
G-C

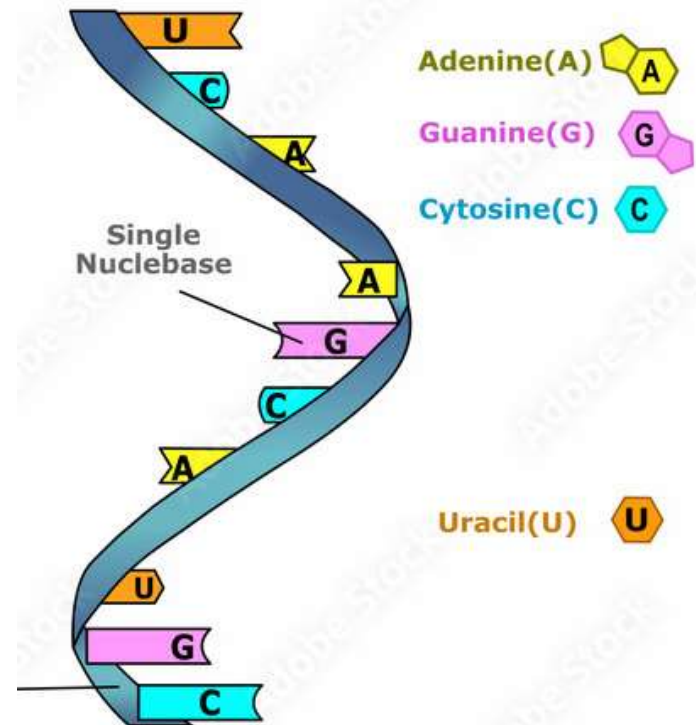
DNA

Deoxyribonucleic Acid



RNA

Ribonucleic Acid

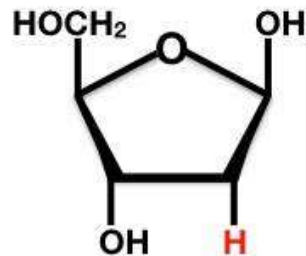


DNA is double-helix, with hydrogen bonds between the nitrogenous bases. DNA stores genetic information.

RNA is single strand. RNA carries DNA information in order to produce proteins.

DNA

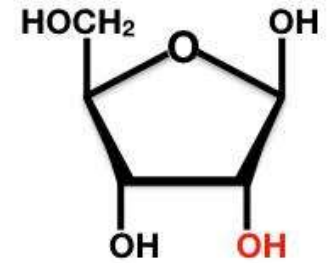
Deoxyribonucleic acid



Deoxyribose

RNA

Ribonucleic acid

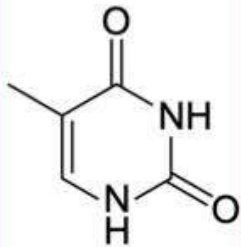


Ribose



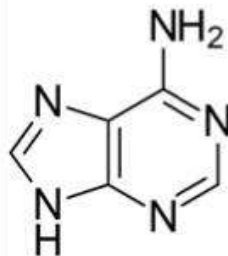
DNA specific nucleobase

THYMINE

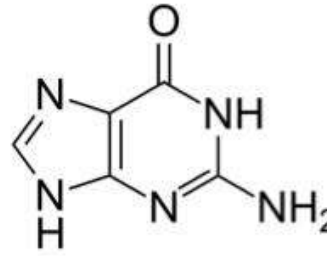


Nucleobases found in DNA and RNA

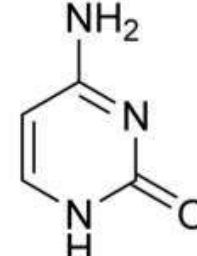
ADENINE



GUANINE



CYTOSINE



RNA specific nucleobase

URACIL

