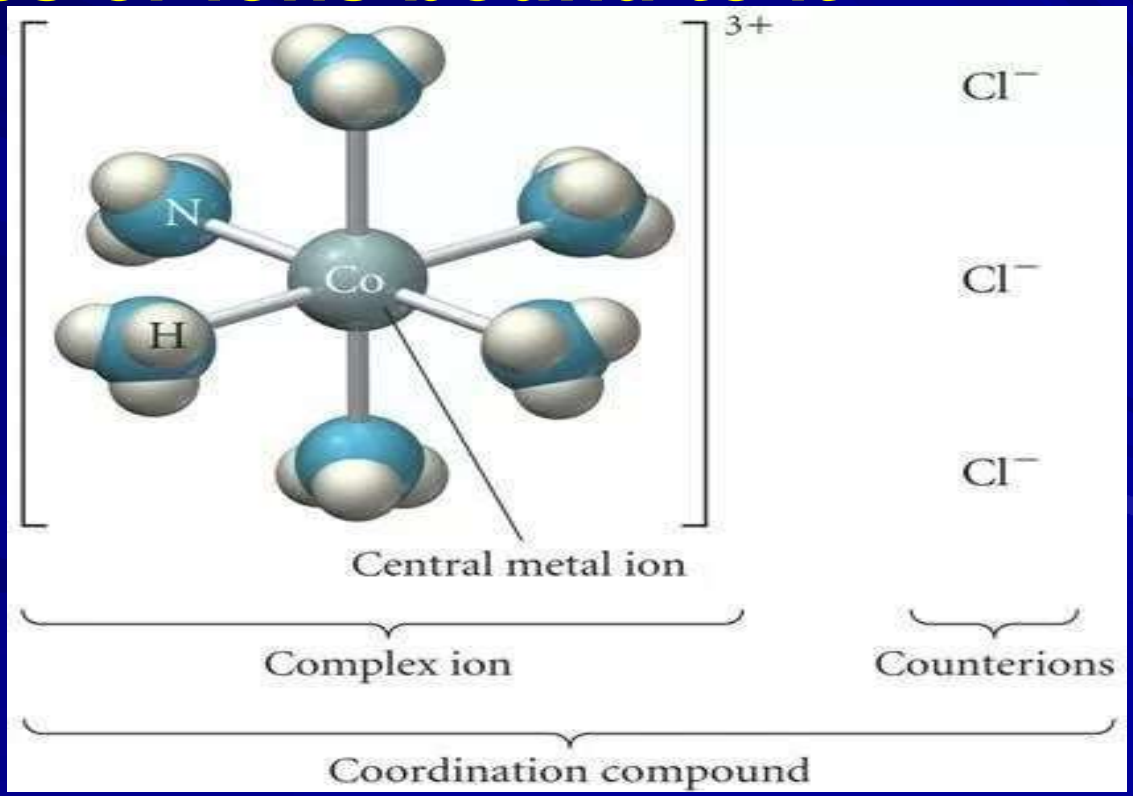
Coordination compounds

Biocomplexes

Medical Chemistry

Coordination compounds

In the crystal lattice, coordination compounds have stable complex ions that consist of a metal ion in the center and molecules or ions bound to it



Importance of coordination compounds in the organism

1. Catalysis

Example: cytochromes, carbanhydrase

2.Oxygen transport and storage

Example: hemoglobin, myoglobin

3.Changes of structure and chemical reactivity

Example: zinc binding to insulin

Structure of coordination compounds

$K_4[Fe(CN)_6]$ potassium hexacyanoferrate

Central atom is Fe^{2+}

Ligands are CN^-

Coordination number is 6

Internal sphere is $[Fe(CN)_6]^{4-}$

Brackets denote covalent bonding

External sphere is $4K^+$

Oxidation state of iron is +2

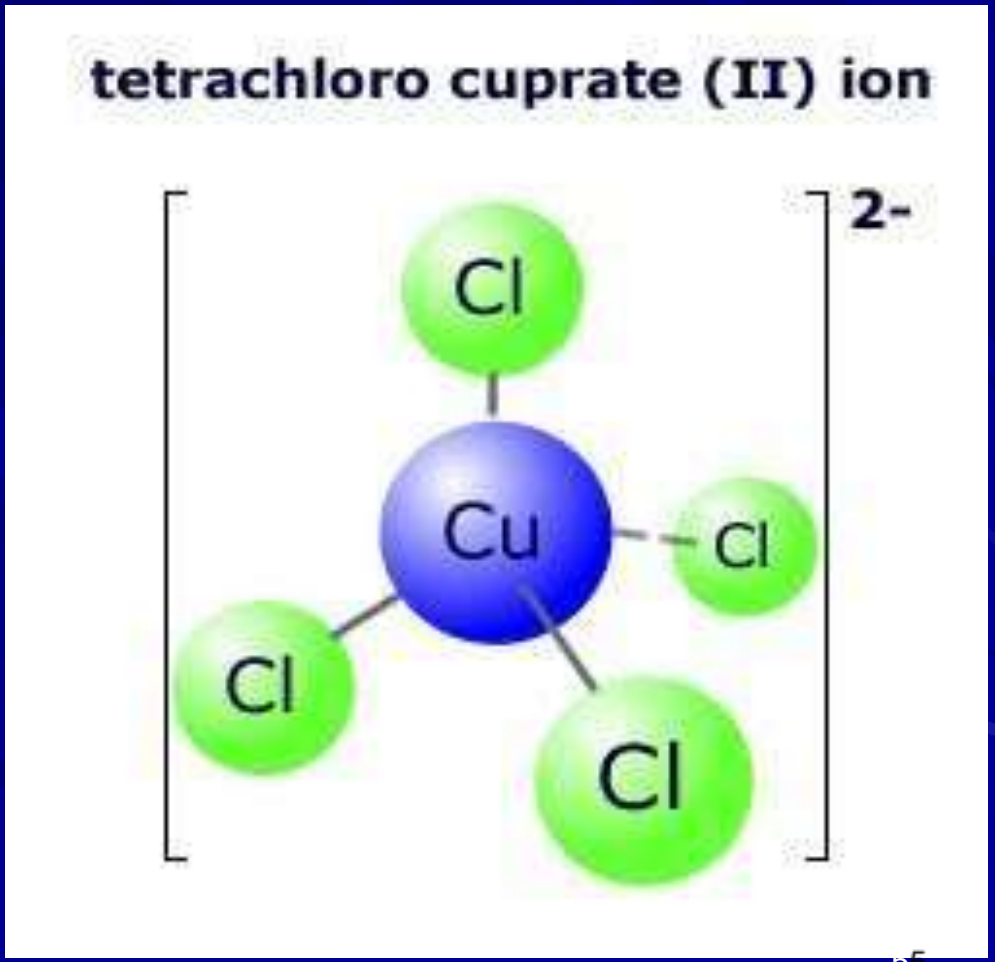
Structure of coordination compounds

Central atom is …

Ligands are …

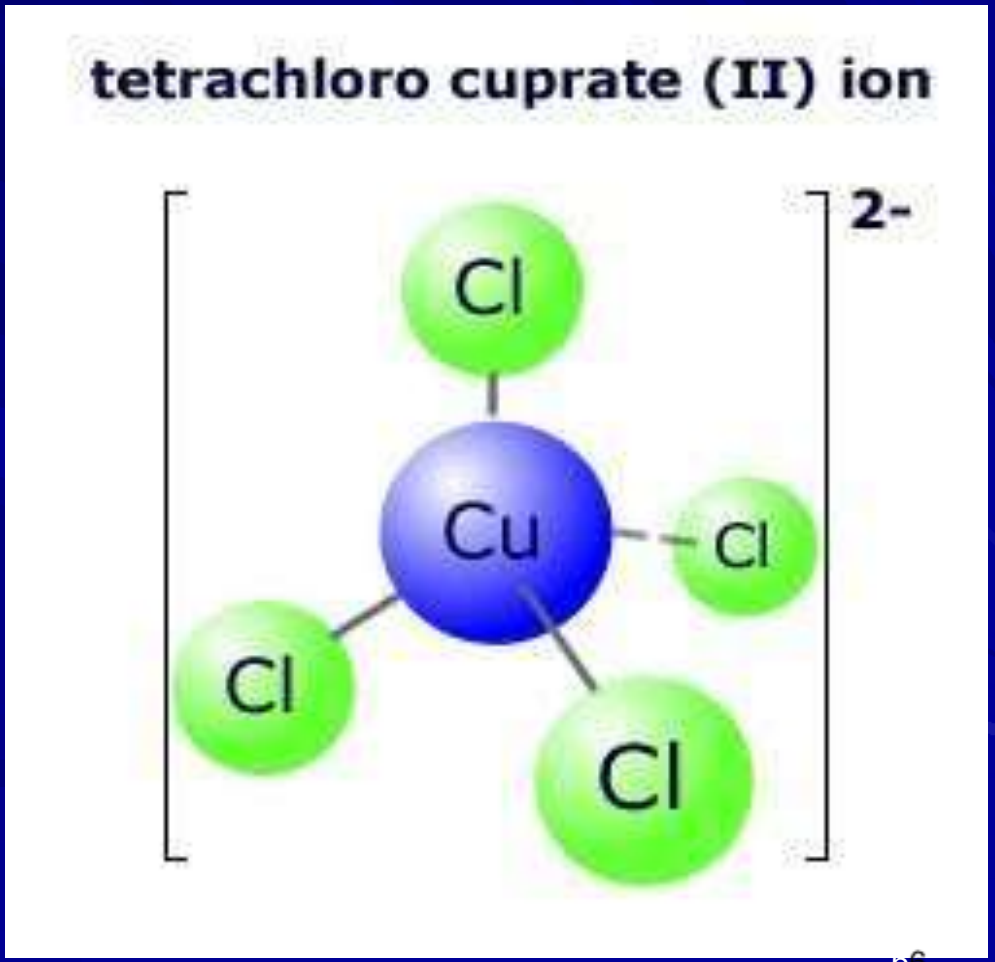
Coordination number is …

Oxidation state of copper is …



Structure of coordination compounds

- Central atom is Cu^{2+}
- Ligands are Cl^-
- Coordination number is 4
- Oxidation state of copper is +2



The central atom

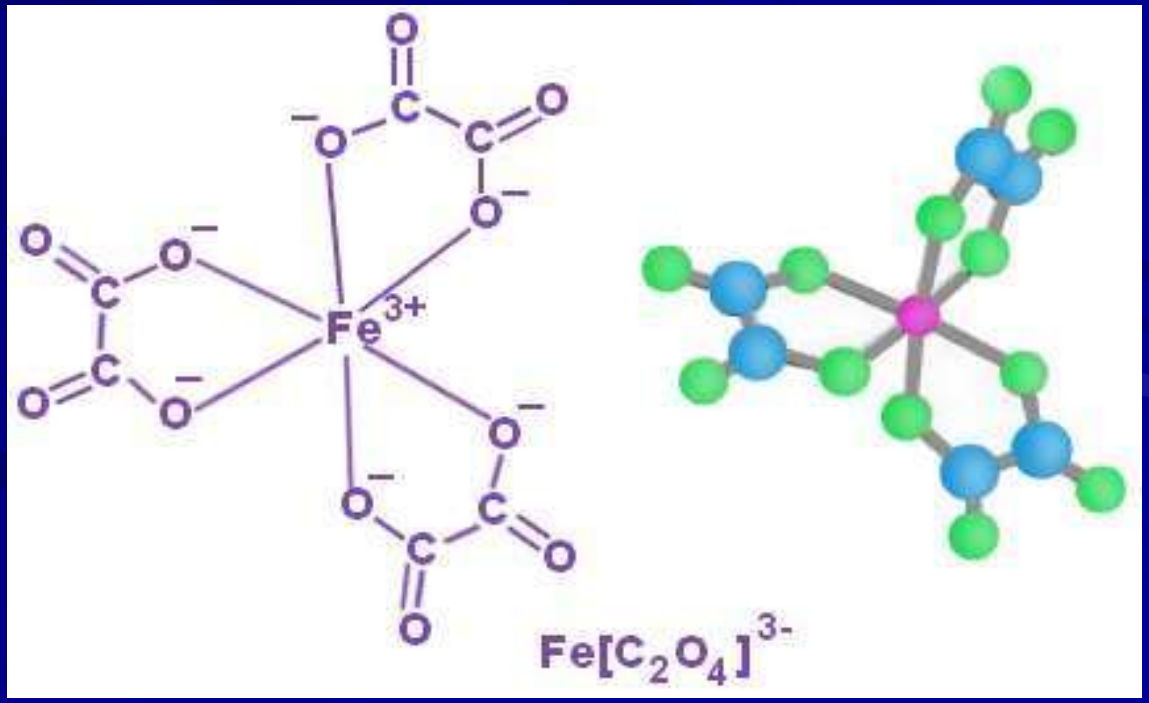
- The central atom is a metal, very often a *d*-block element
- In a complex ion, the central atom forms more bonds than is allowed by its valency

Ligands

- Ligands can be either molecules or ions.
- Ligands have denticity. Denticity is the number of bonds between the ligand and the central atom
- Monodentate ligands – one bond
- Bidentate ligands – two bonds
- Polydentate ligands – several bonds, often chelate ligands
- Chelate ligands – two or more bonds

Coordination number

- Coordination number is the number of bonds between the central atom and the ligands
- Most often, it is 4 and 6



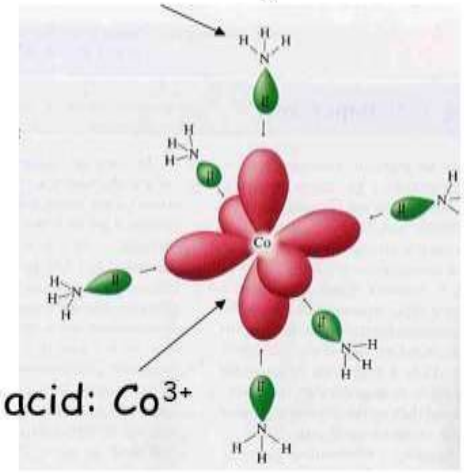
Bonding in coordination complexes

The mechanism is donor-acceptor.

The resulting bond is polar covalent.

The formation of a coordinate complex is a ***Lewis acid-base*** reaction

Lewis base: $:NH_3$



Lewis acid: Co^{3+}

Coordination complex: Lewis base (electron pair donor) coordinated to a Lewis acid (electron pair acceptor)

Coordination complex: Ligand (electron donor) coordinated to a metal (electron acceptor)

The number of ligand bonds to the central metal atom is termed the coordination number

6

Classification of coordination complexes by the charge of the complex ion

1. …

Example: $[Zn(NH_3)_4]SO_4$

2. …

Example: $Na_3[Al(OH)_6]$

3. …

Example: $Fe(CO)_5$

Classification of coordination complexes by the charge of the complex ion

1. Cationic

Example: $[Zn(NH_3)_4]SO_4$

2. Anionic

Example: $Na_3[Al(OH)_6]$

3.Neutral

Example: $Fe(CO)_5$

Classification of coordination complexes by the identity of the ligands

1. …

Example: $[Ag(NH_3)_2]Cl$, $Co_2(CO)_8$

2. …

Example: $K_3[Cr(OH)_6]$, $K_2[HgI_4]$

3. …

Example: $Pt(NH_3)_2Br_2$

Classification of coordination complexes by the identity of the ligands

1. Molecular

Example: $[Ag(NH_3)_2]Cl$, $Co_2(CO)_8$

2. Ionic

Example: $K_3[Cr(OH)_6]$, $K_2[HgI_4]$

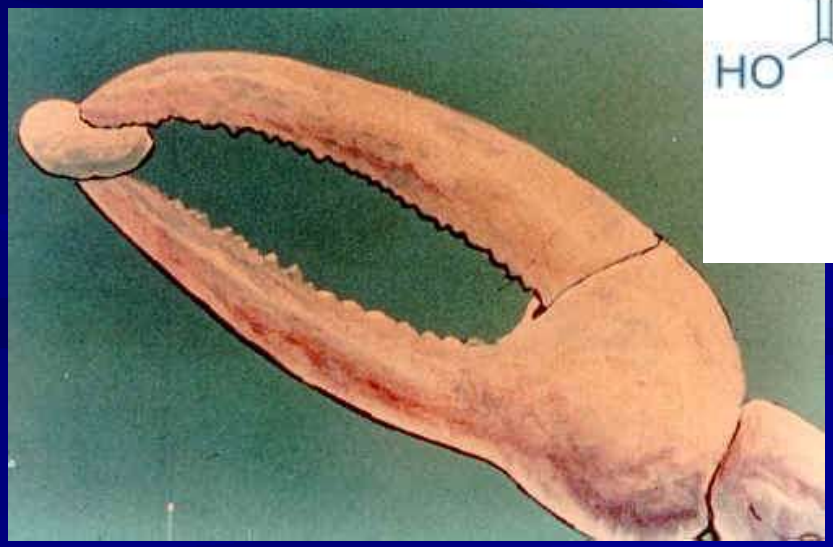
3. Mixed

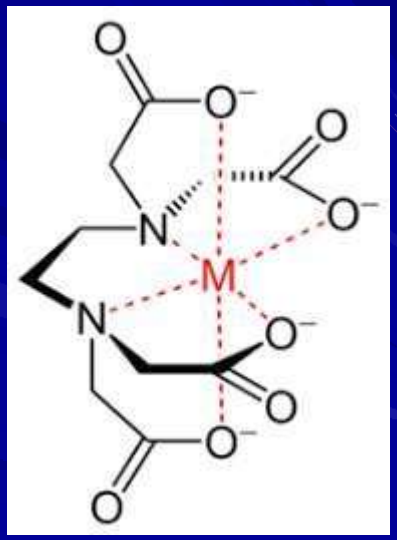
Example: $Pt(NH_3)_2Br_2$

Chelation

Chelation is formation of several bonds between an organic molecule and a metal atom. Example:

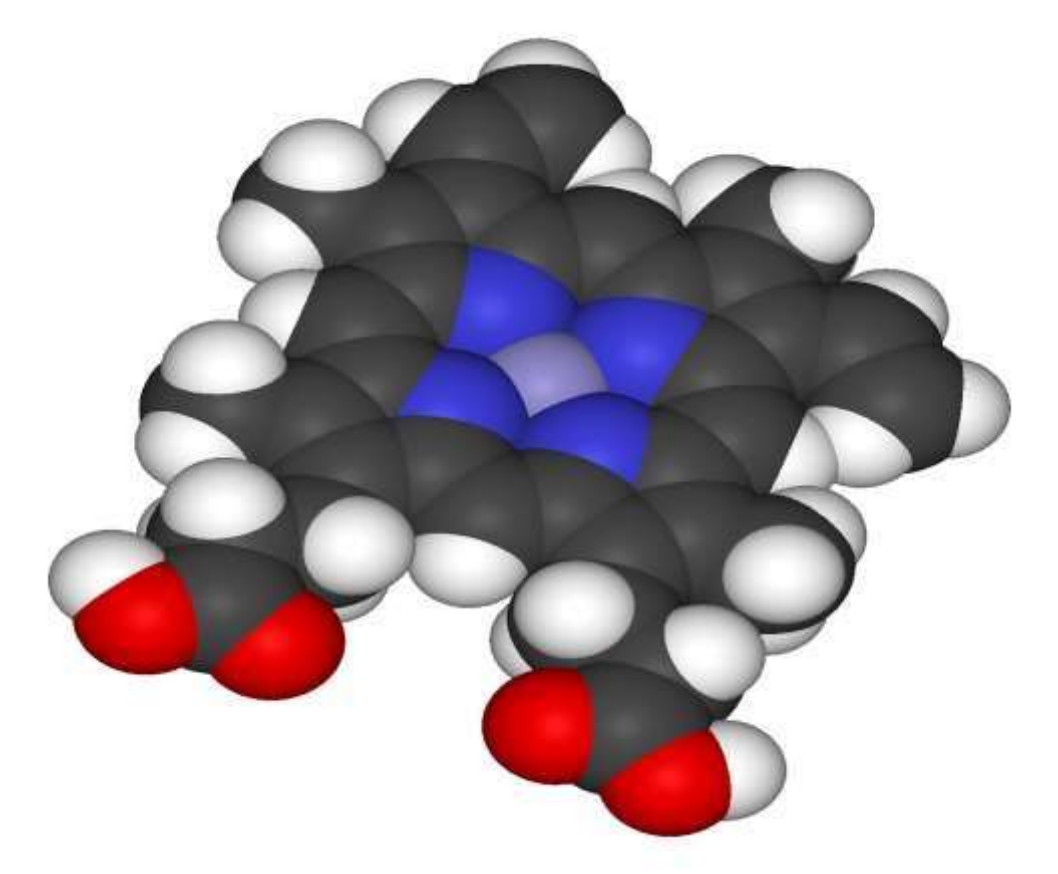
Disodium ethylenediaminetetraacetic acid (EDTA)





Chelation

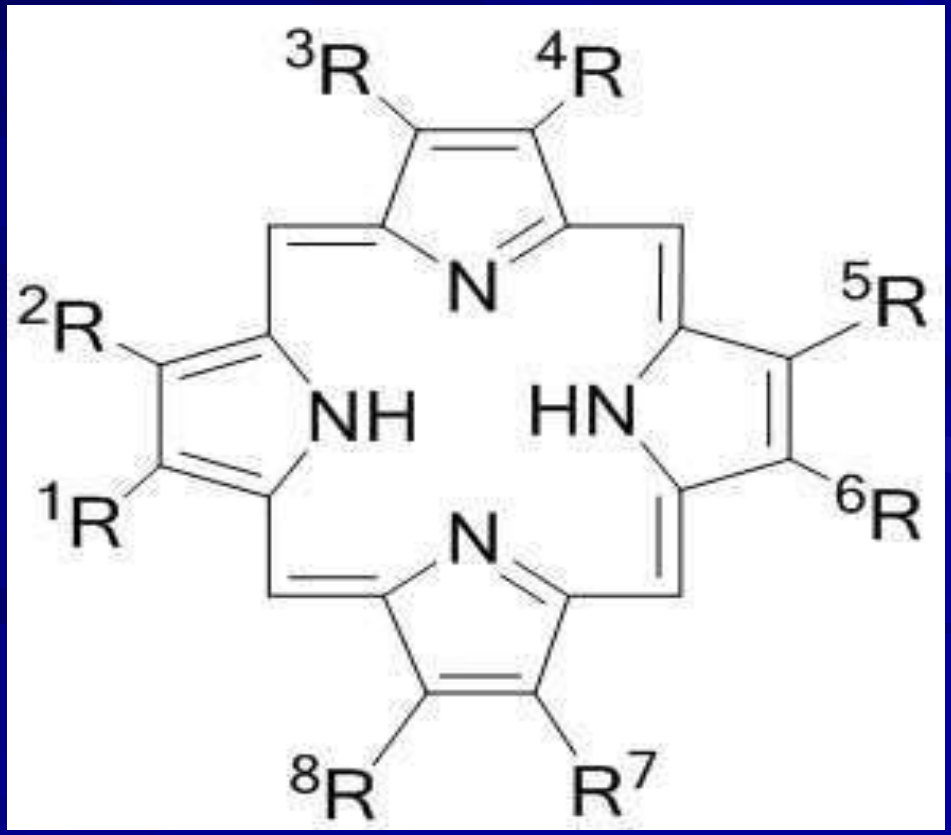
Main property of chelates is extra stability, e.g. in the heme:



Chelating ligands in the organism

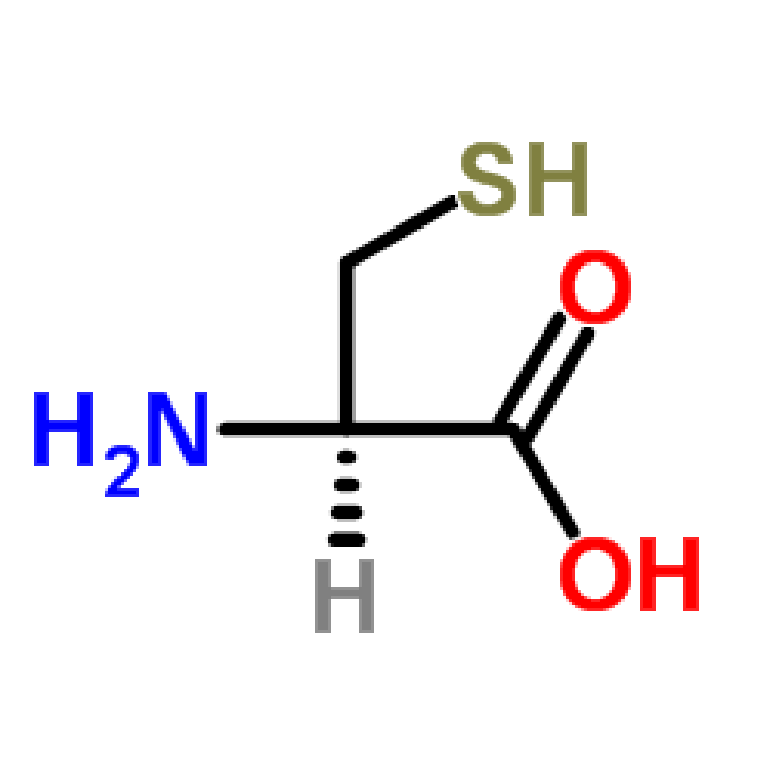
- **Macrocycles**

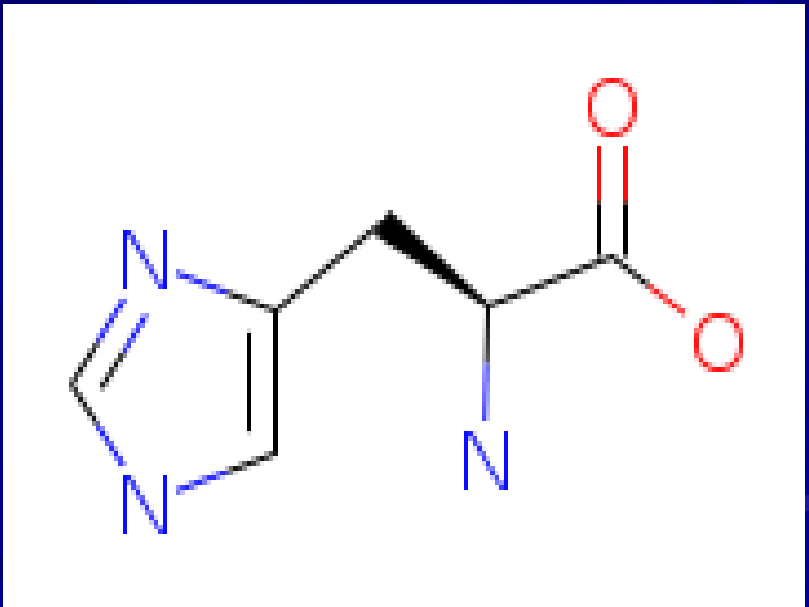
  (e.g. porphyrin, corrin rings)



Chelating ligands in the organism

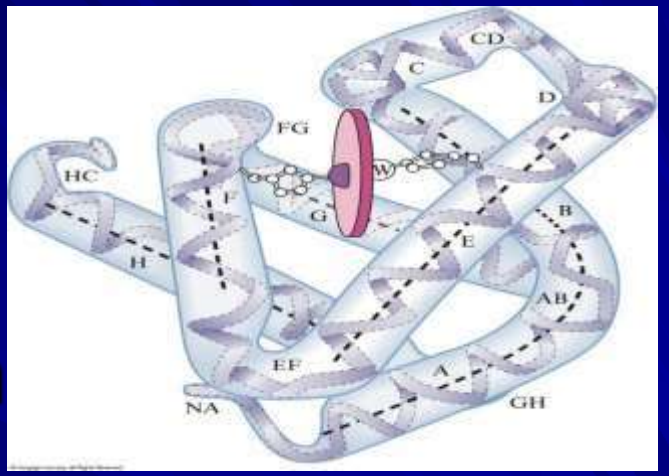
- **Amino acid residues in proteins (e.g. cysteine, histidine)**





Biocomplexes of iron.

Heme proteins. Myoglobin



Structure: one chain

Location: muscle

Role: a reservoir for oxygen

and an oxygen carrier in muscle cells

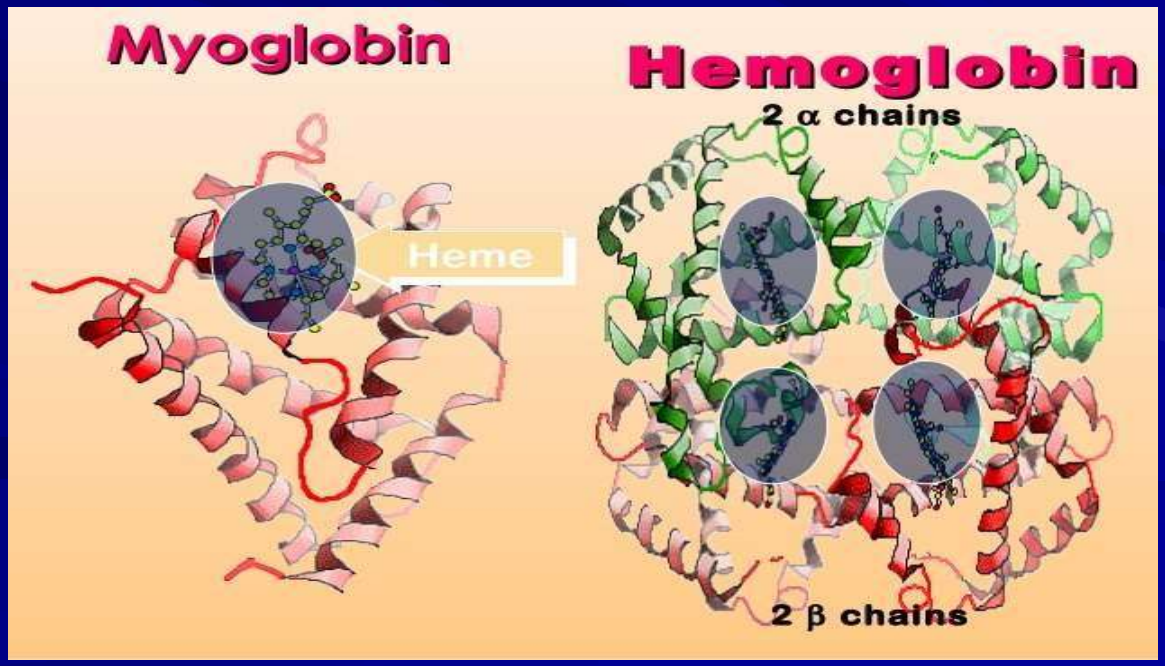
Biocomplexes of iron.

Heme proteins. Hemoglobin

Structure: four chains

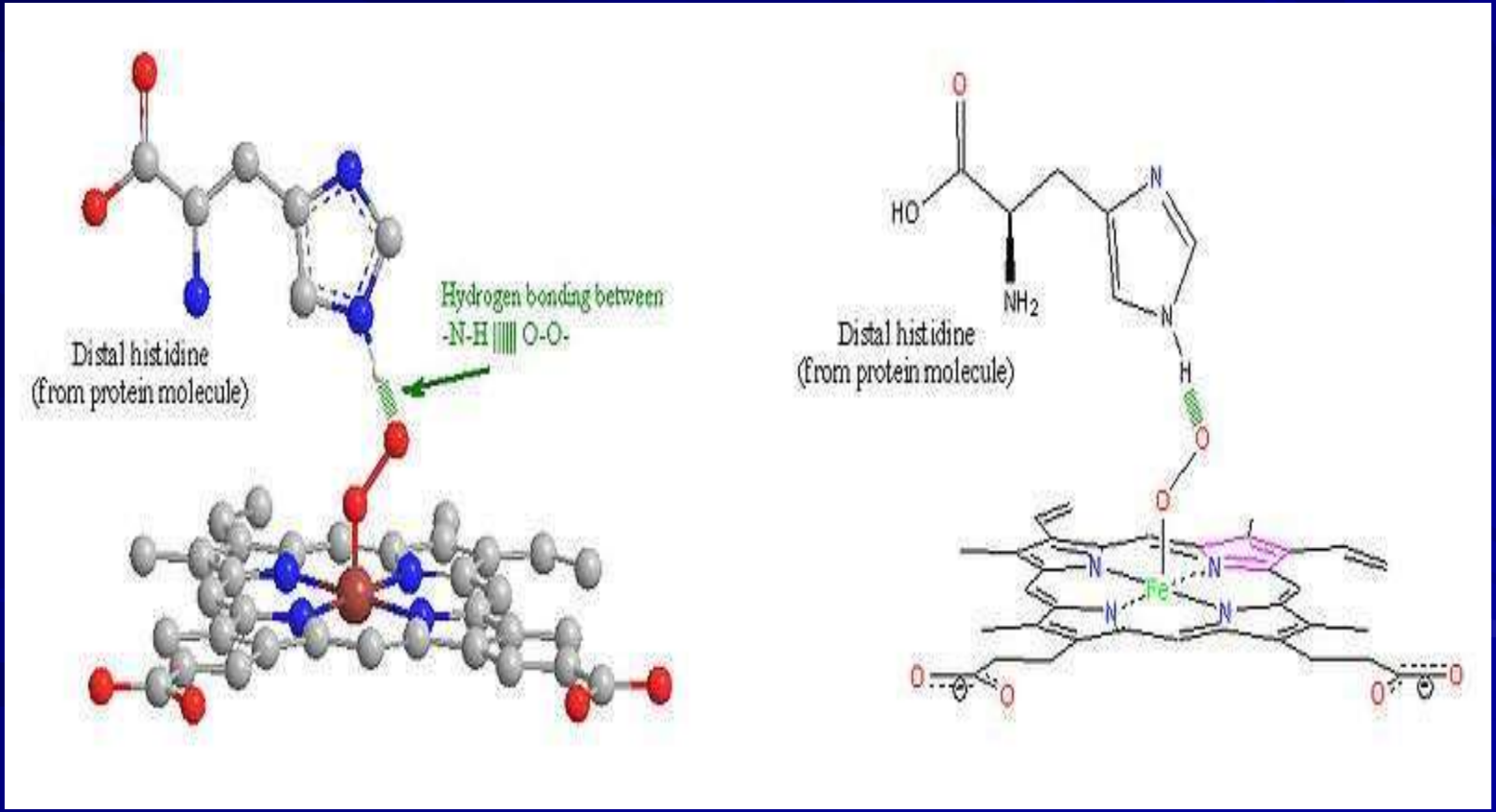
Location: red blood cells

Role: transport of oxygen in blood



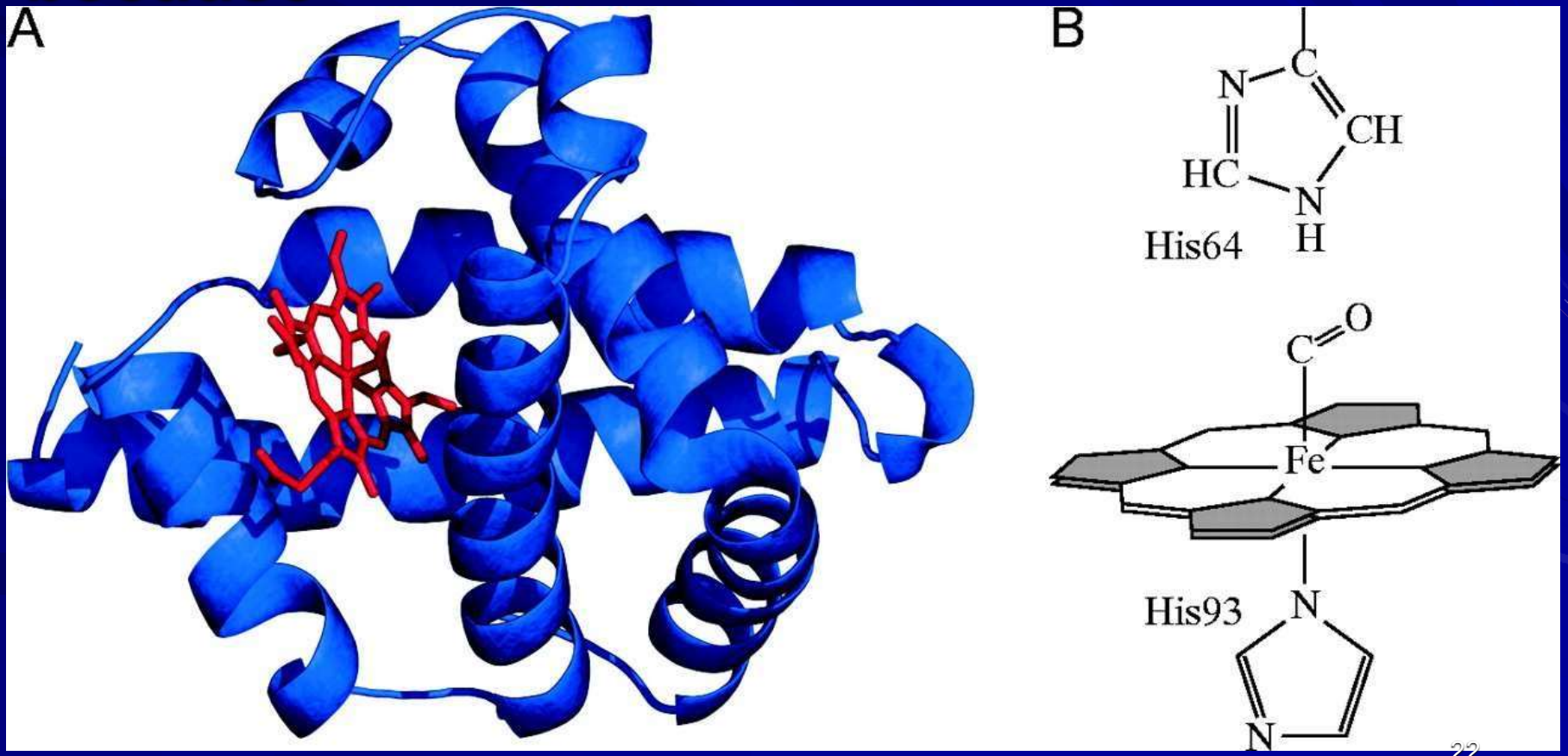
Biocomplexes of iron.
Heme proteins. Hemoglobin

Structure of heme:



Biocomplexes of iron.
Heme proteins. Hemoglobin

Carbon monoxide CO is poisonous because

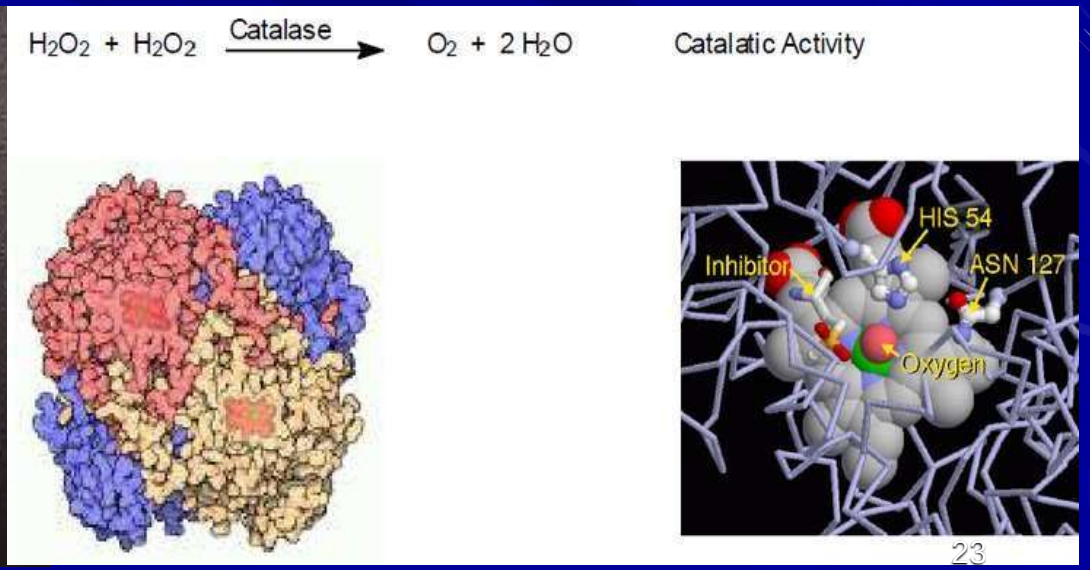


Biocomplexes of iron.
Heme proteins. Catalase

Location: peroxisomes

Role: decomposing of hydrogen peroxide

Structure: four chains

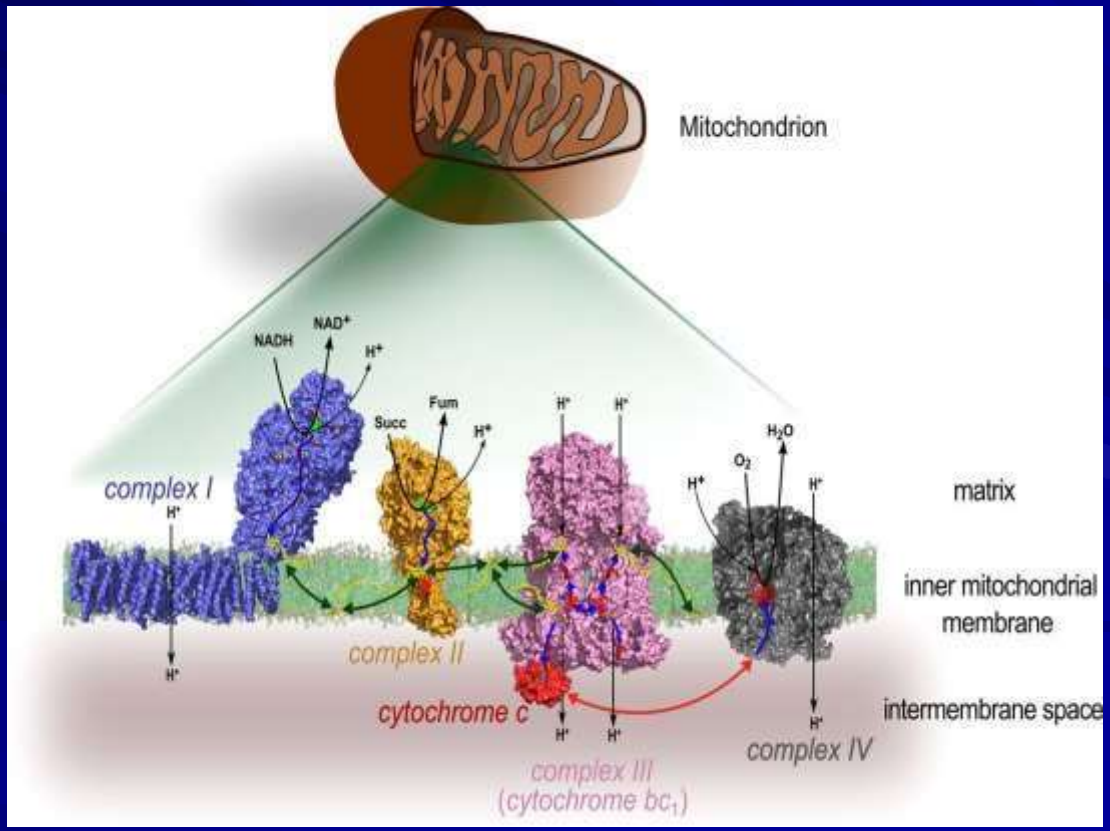


Biocomplexes of iron.

Heme proteins. Cytochromes

Location: mitochondria

Role: transport of electrons

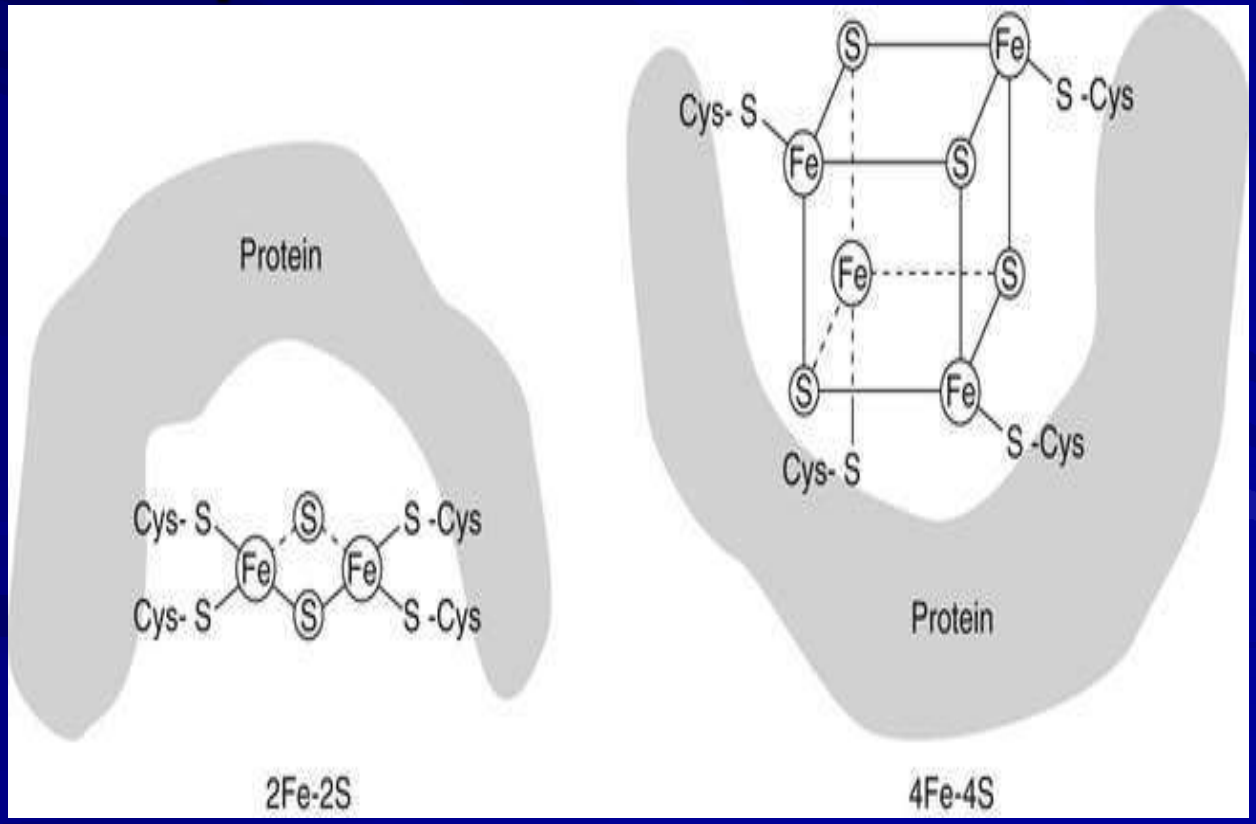


Biocomplexes of iron.

Nonheme proteins. Fe-S proteins

Location: mitochondria

Role: transport of electrons

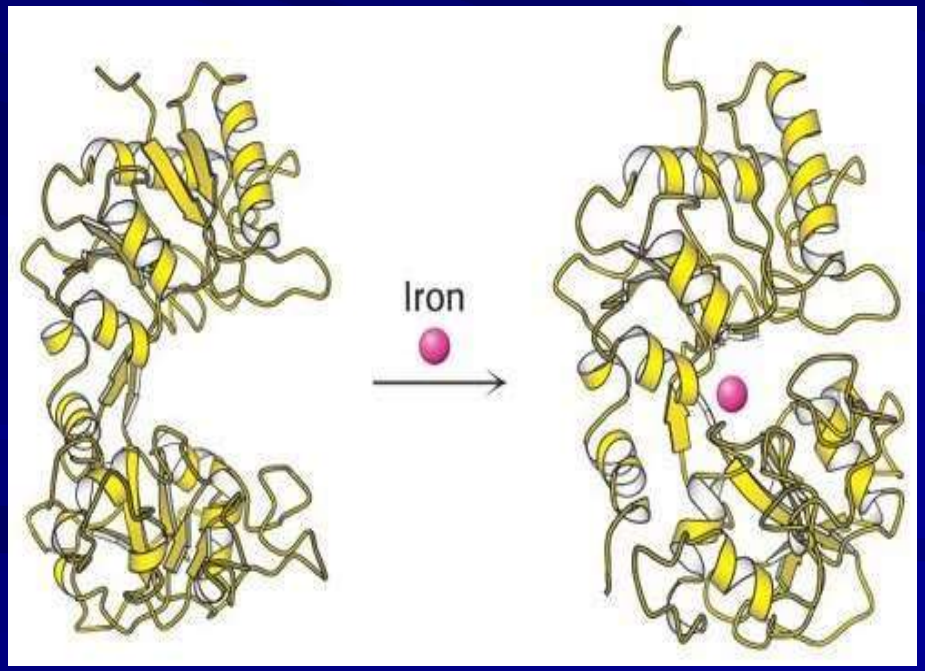


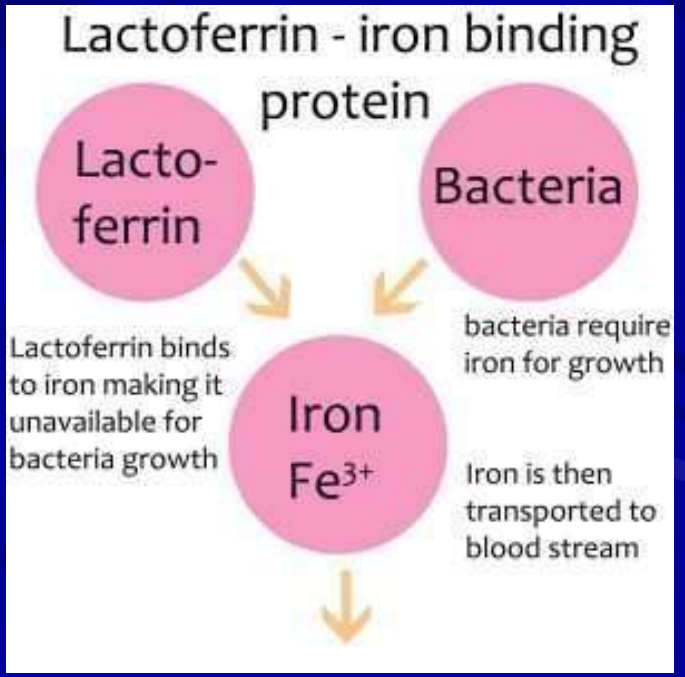
Biocomplexes of iron.

Nonheme proteins. Lactoferrin

Location: secreted fluids

Role: innate immune defense



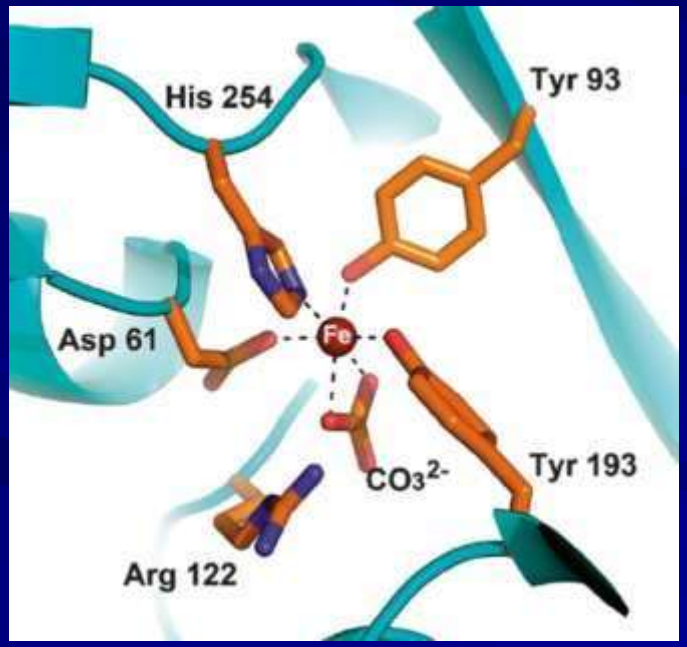


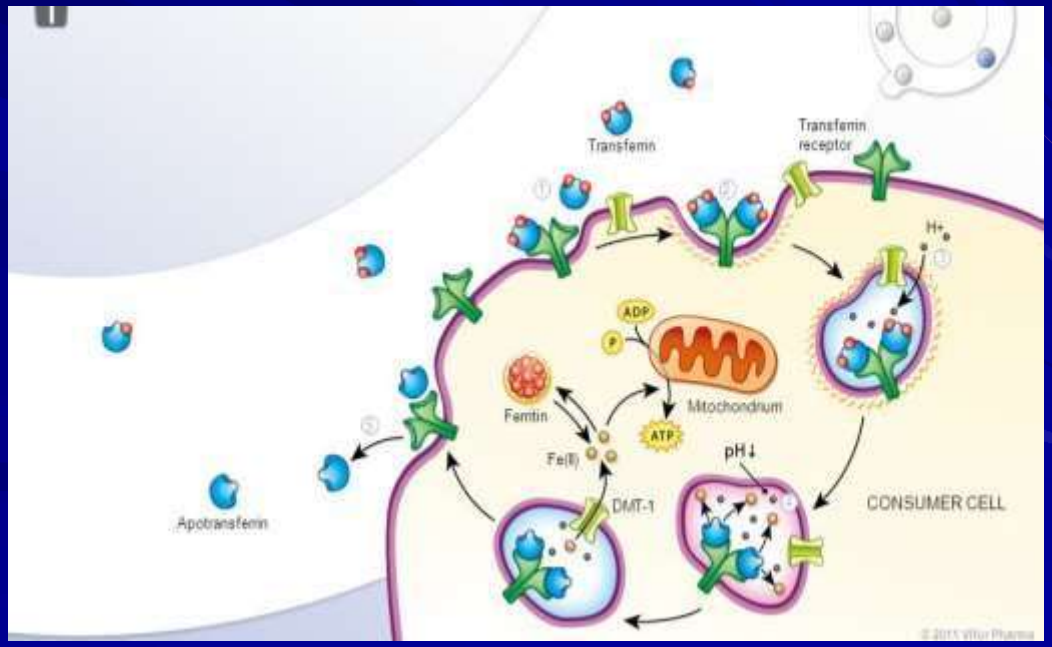
Biocomplexes of iron.

Nonheme proteins. Transferrin

Location: blood plasma

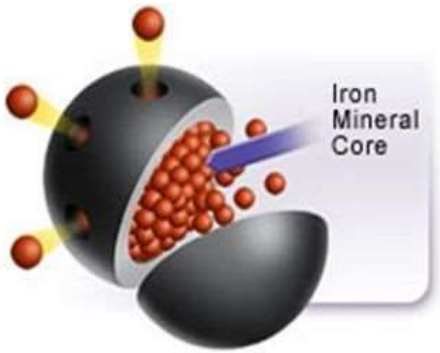
Role: transport of iron



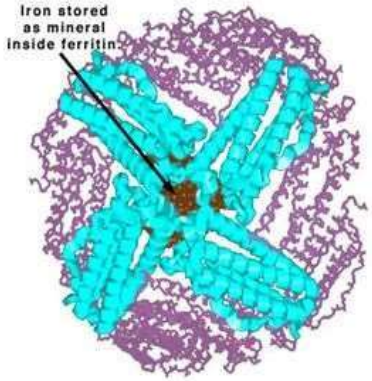


Biocomplexes of iron. Nonheme proteins. Ferritin

- **Iron storage**
  - Iron can be stored by ferritin (a protein) or hemosiderin
    - Stored in liver, bone marrow (why here?), intestinal mucosa, and spleen
    - A apoferritin molecule can combine with 4,000 atoms of iron.



Ferritin

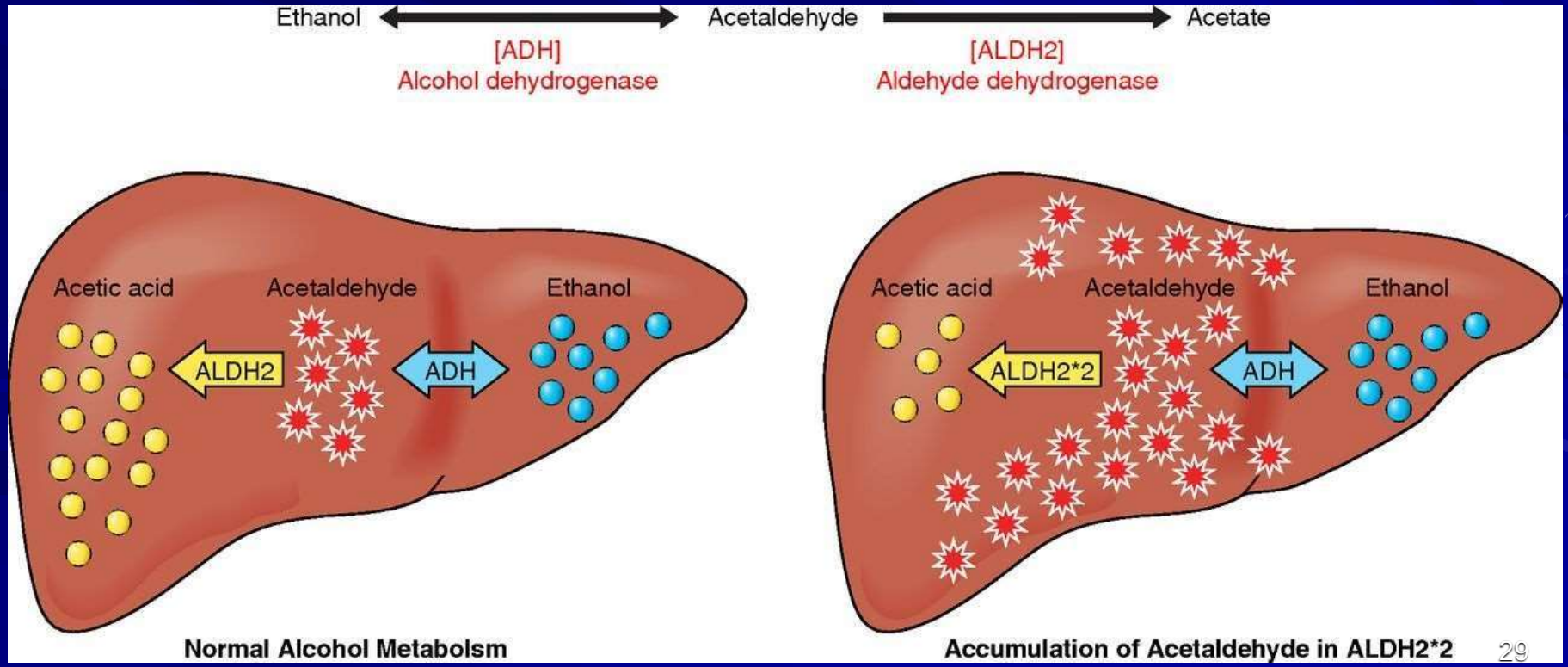


Ferritin

Biocomplexes of zinc. Alcohol dehydrogenase

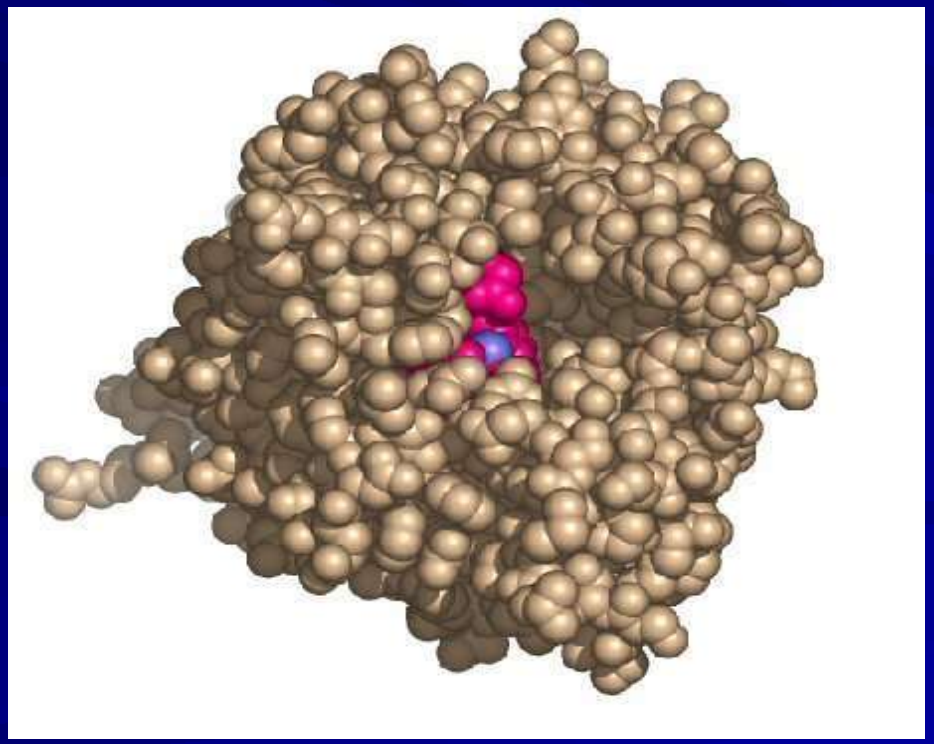
Location: liver

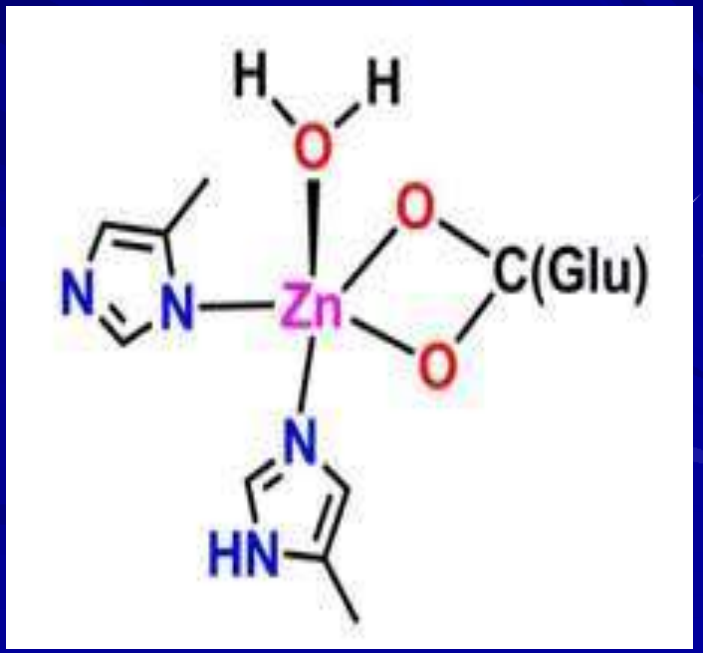
Role: oxidation of ethanol to ethanal



Biocomplexes of zinc.
Carboxypeptidase

Role: a protease that hydrolyzes a peptide bond at the C–terminal end of a protein.

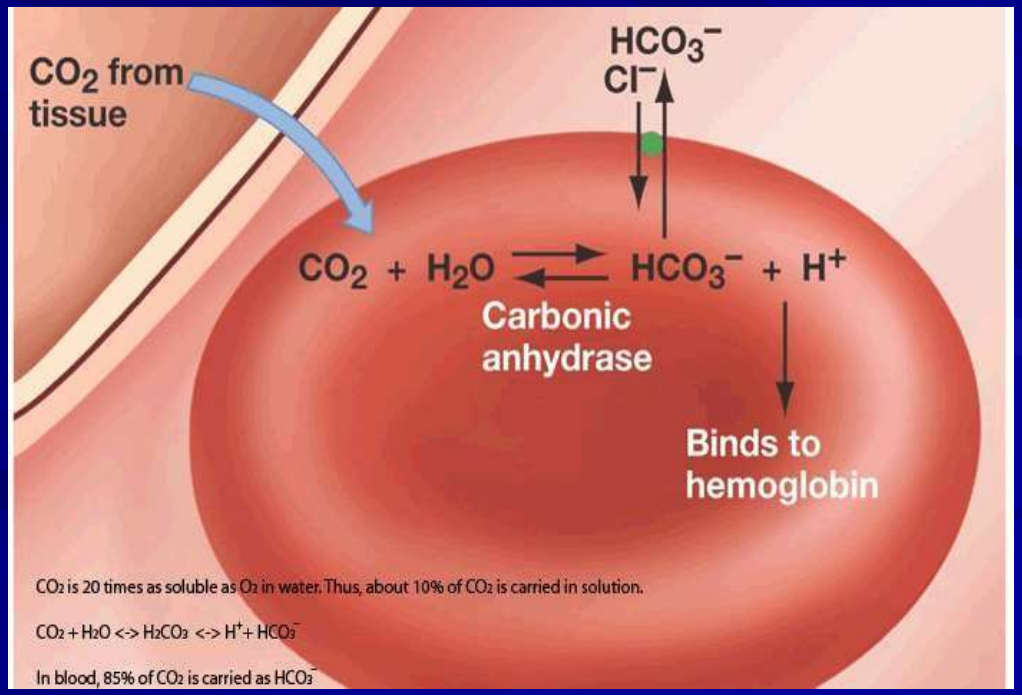




Biocomplexes of zinc. Carbonyc anhydrase

Location: red blood cells

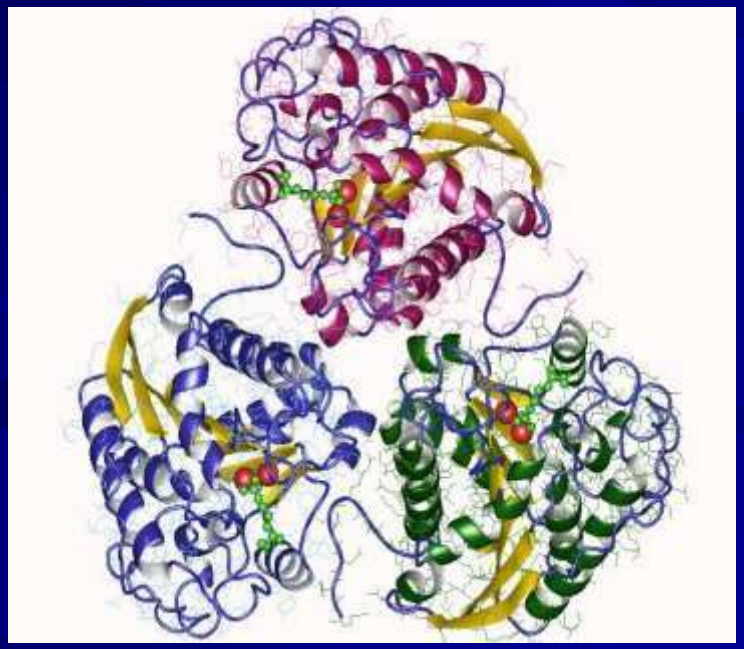
Role: formation of carbonic acid and bicarbonate buffer system

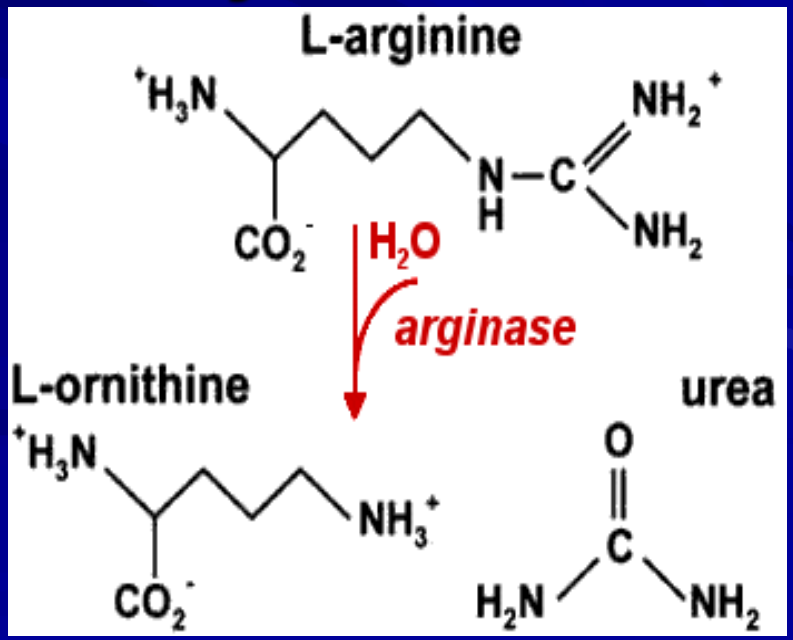


Biocomplexes of manganese. Arginase

Location: liver

Role: converts the amino acid arginine to ornithine and urea H2N–CO–NH2 in the final reaction of the urea cycle.





Biocomplexes of copper. Ceruloplasmin

Location: blood plasma

Role: it oxidizes Fe^{+2} to Fe^{+3} to make it ready for transportation in blood