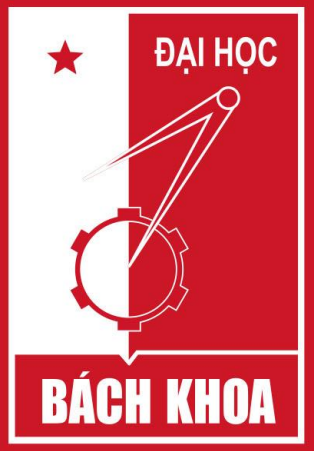


ĐẠI HỌC BÁCH KHOA HÀ NỘI
VIỆN CÔNG NGHỆ THÔNG TIN VÀ TRUYỀN THÔNG

School of Information and Communication Technology
Hanoi University of Science and Technology

Bioinformatics: Theory and Applications

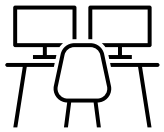
Dr. Quang H. Nguyen
Head of Bioinformatics Lab
BK.AI

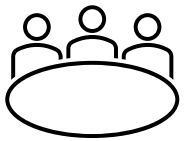
3th June 2021

Contents

- Energy and nutrition
- Role of enzymes and hormones
- Central Dogma
- Main research topics
  - Gene Regulation
  - Immune system
  - Drug Discovery

Energy and nutrition





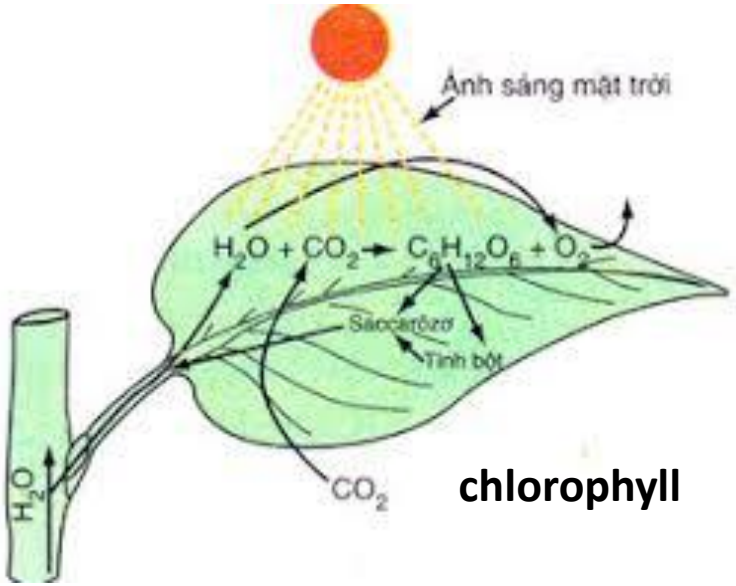
Starch (Tinh bột)
Fat (Chất béo)
Protein
Vitamin
Muối khoáng
(Mineral Salt)

Digestive system and photosynthesis

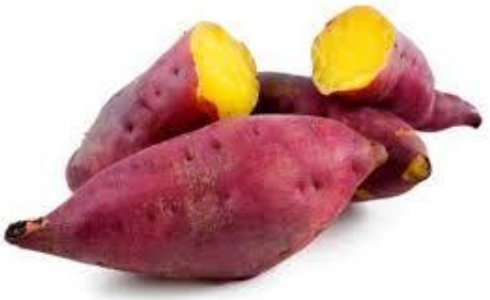
năng lượng ánh sáng mặt trời

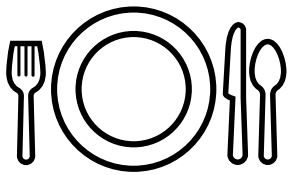
$$6CO_2 + 6H_2O \xrightarrow{\text{được diệp lục hấp thụ}} C_6H_{12}O_6 + 6O_2$$

khí cacbonic — nước — glucoz — oxy



chlorophyll



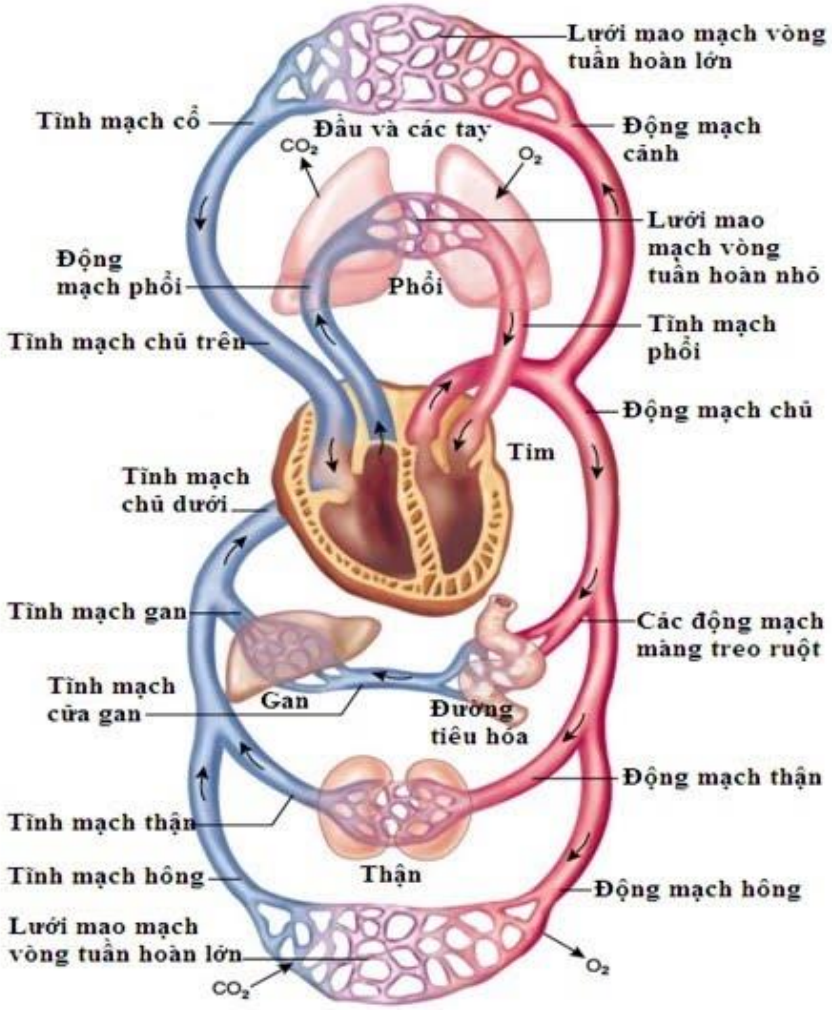


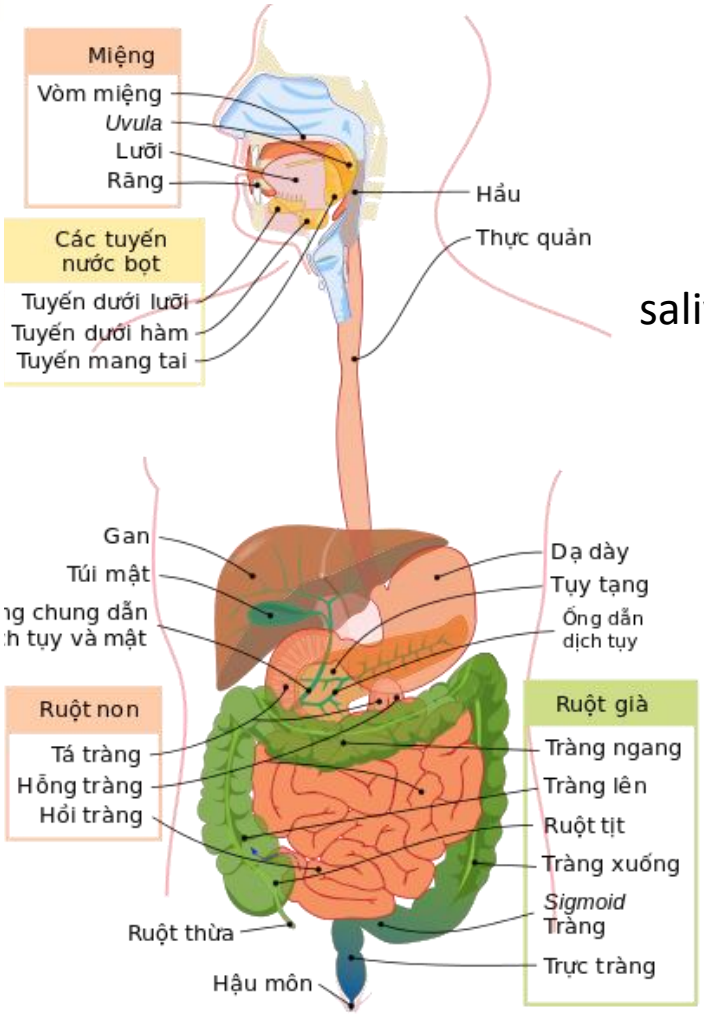
$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

glucoz — oxy — dioxit cacbon — nước

$\Delta G = -2870 kJ/mol$

Circulatory system and digestive system (Hệ tuần hoàn và hệ tiêu hóa)





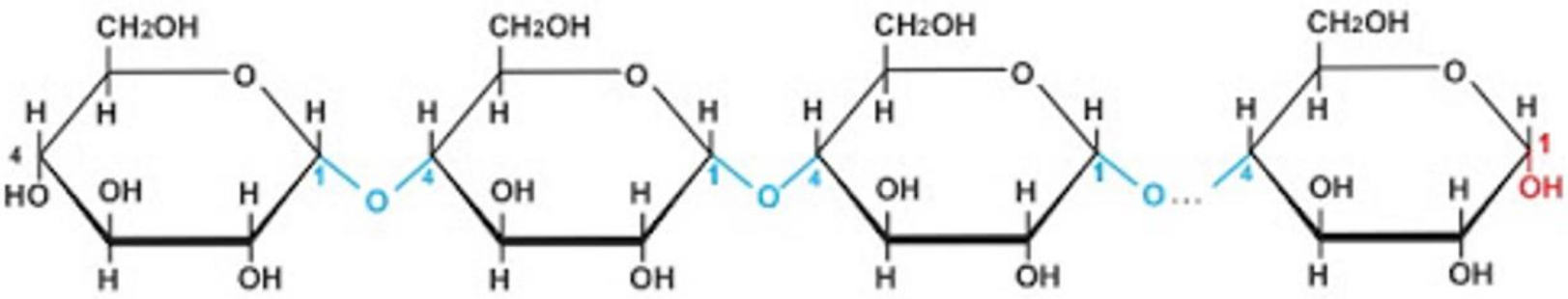
enzyme amylase

salivary glands

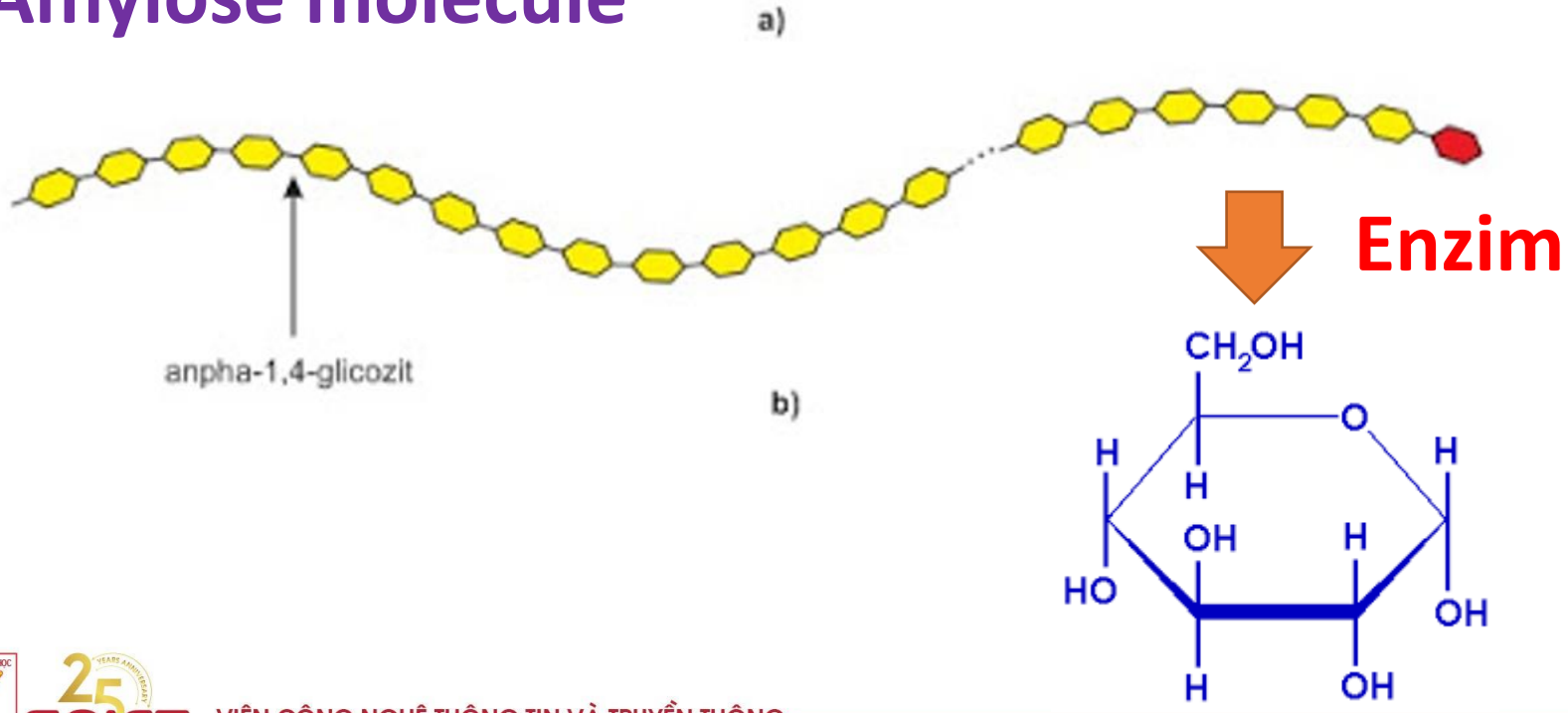
gastric juice (dịch vị) HCl

small intestine (ruột non)

Role of enzyme amylaza

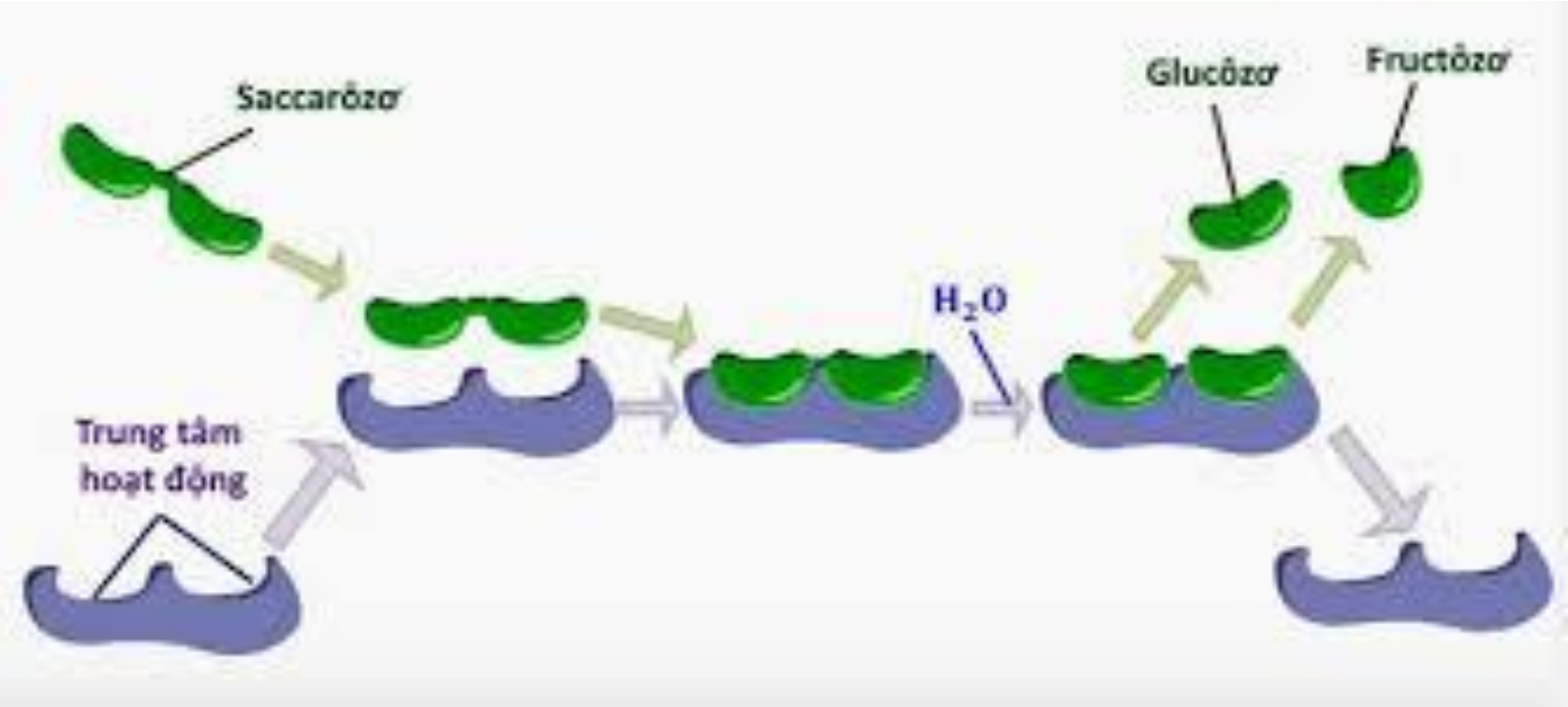


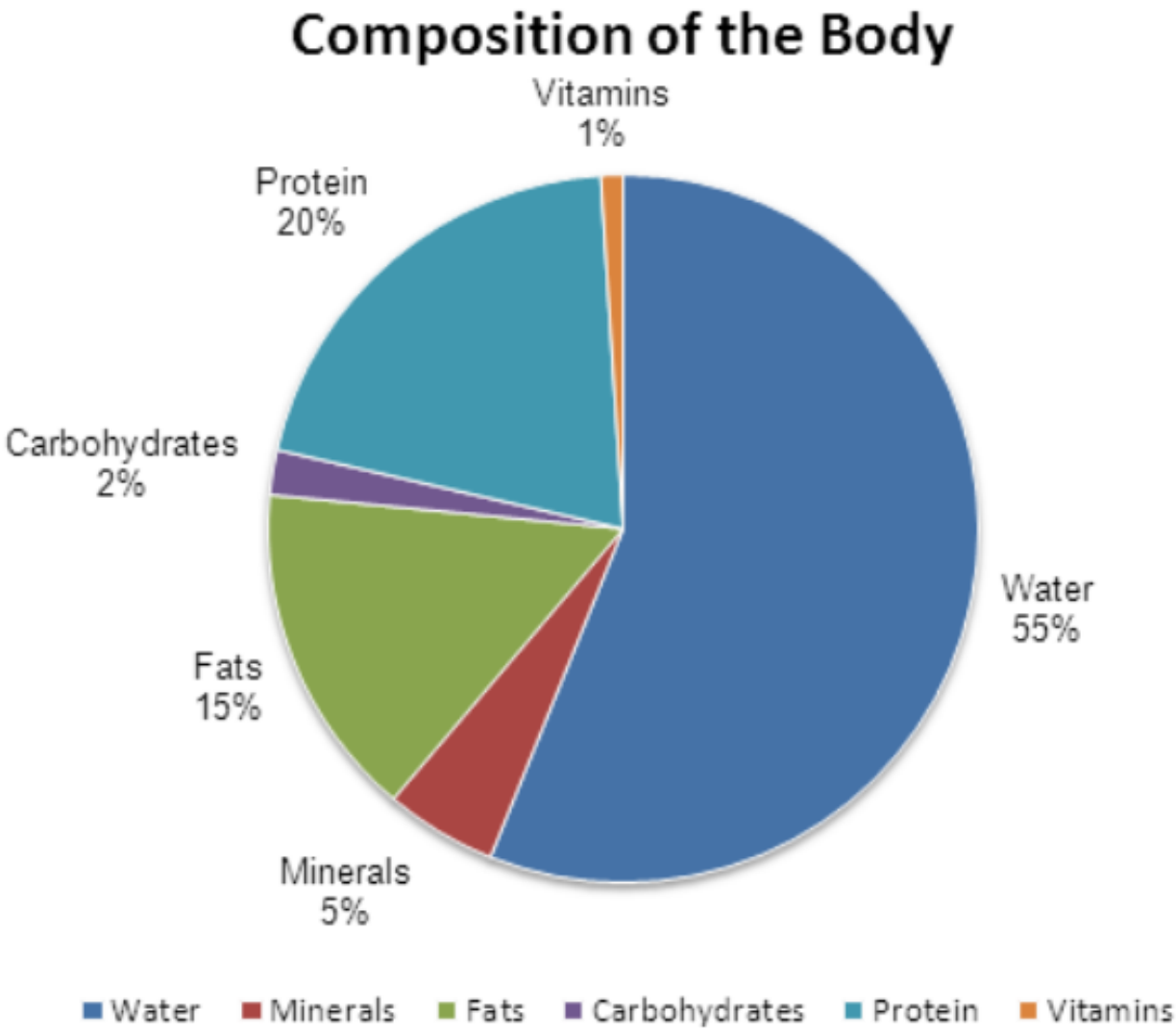
Amylose molecule



The role of enzymes

- Enzyme is a protein, which acts as a catalyst to speed up the reaction.

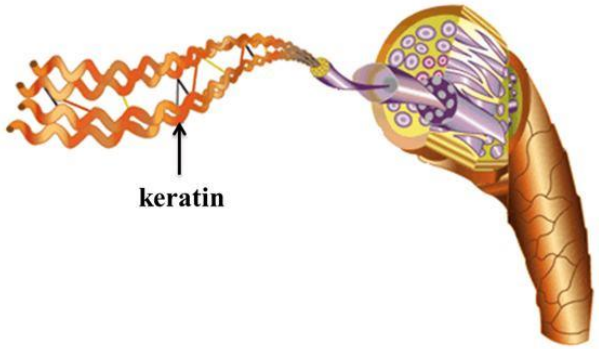


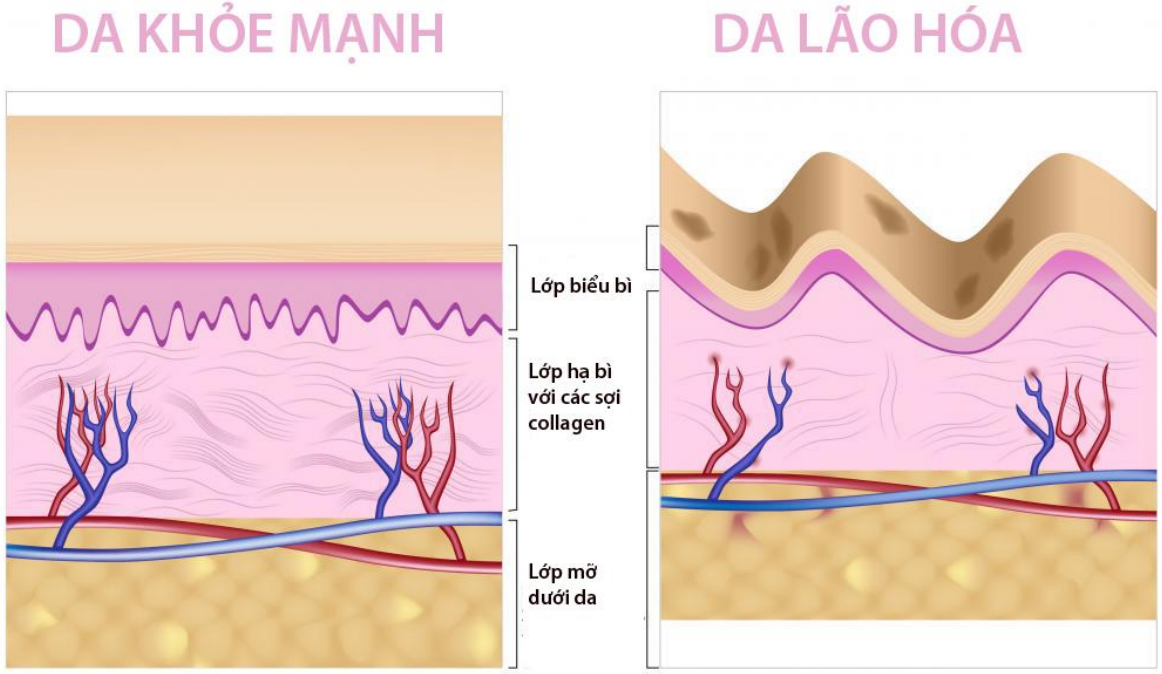


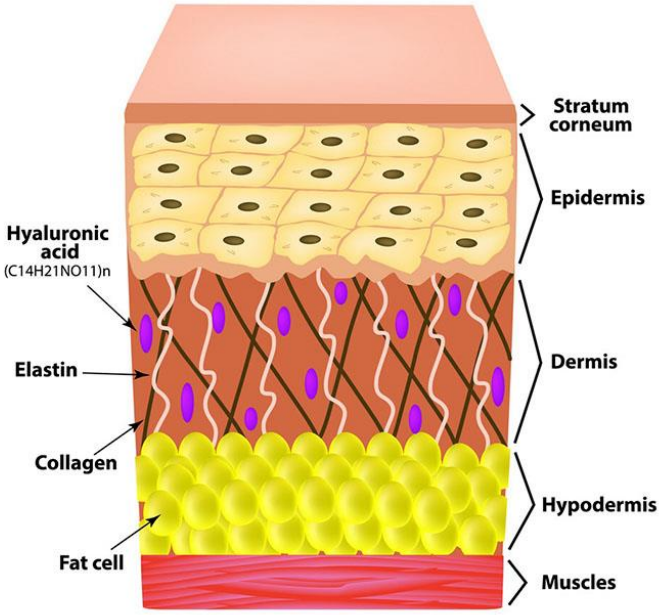
https://radianthealthclub.com/composition-of-the-human-body/

Roles and functions of proteins
a. Body and Cell Structure - Fibrous Proteins

- Collagen and elastin: the main proteins of skin and connective tissue
- Keratin: in hair, horns, nails and feathers







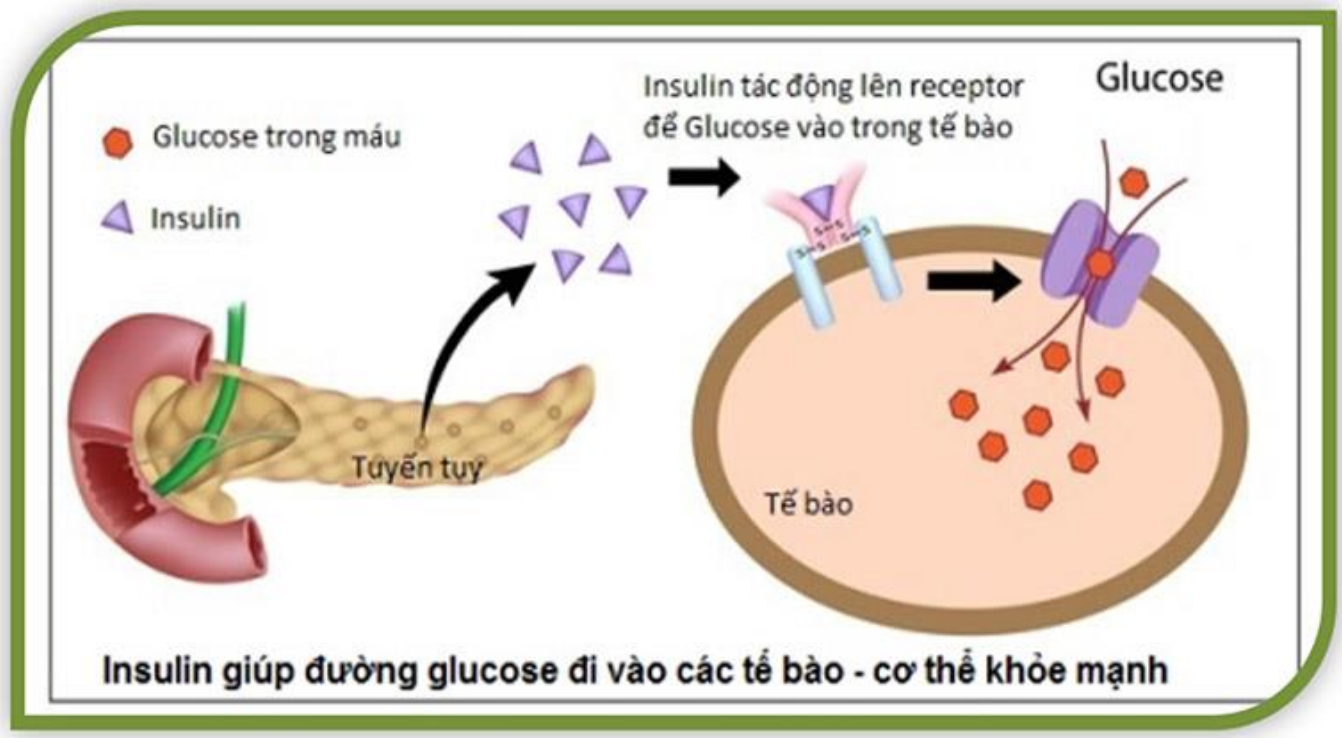
Roles and functions of proteins
b. Protein granules

- These proteins are easily soluble in water.
- As the main active protein of metabolism
- Used as enzymes, hormones, antibodies, clotting agents...

Amylase is an enzyme found in the saliva of humans and some animals that catalyzes the hydrolysis of starch

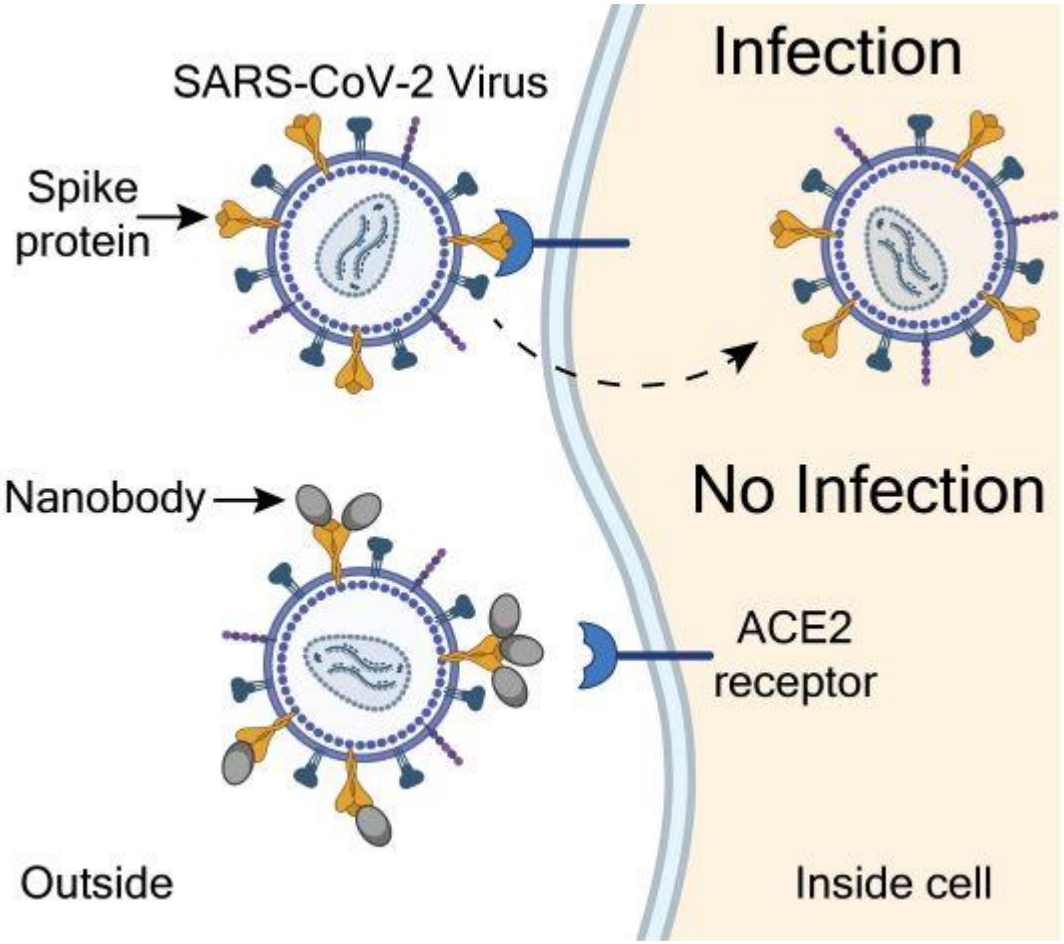
Properties and roles of hormones

- Example: Insulin is a hormone produced by cells in the pancreas.

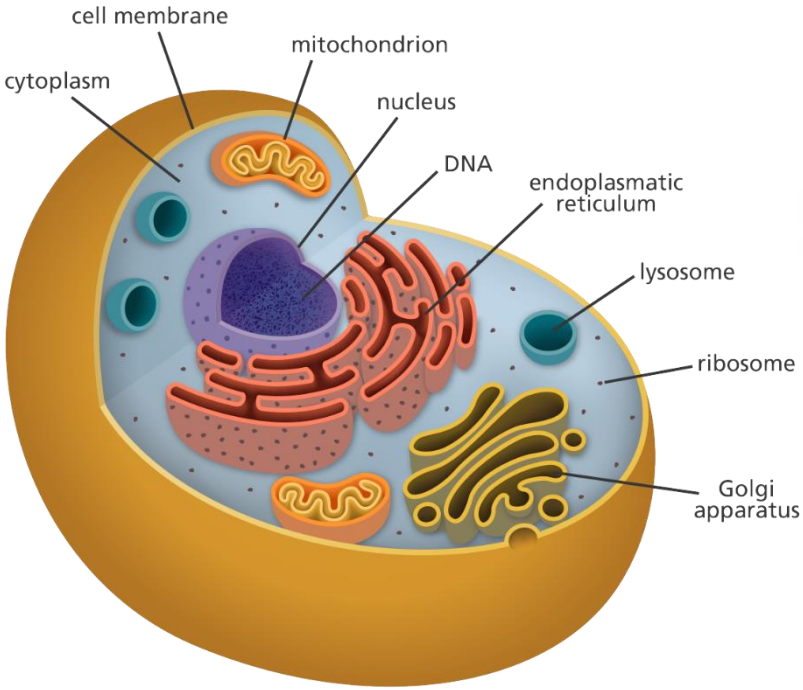


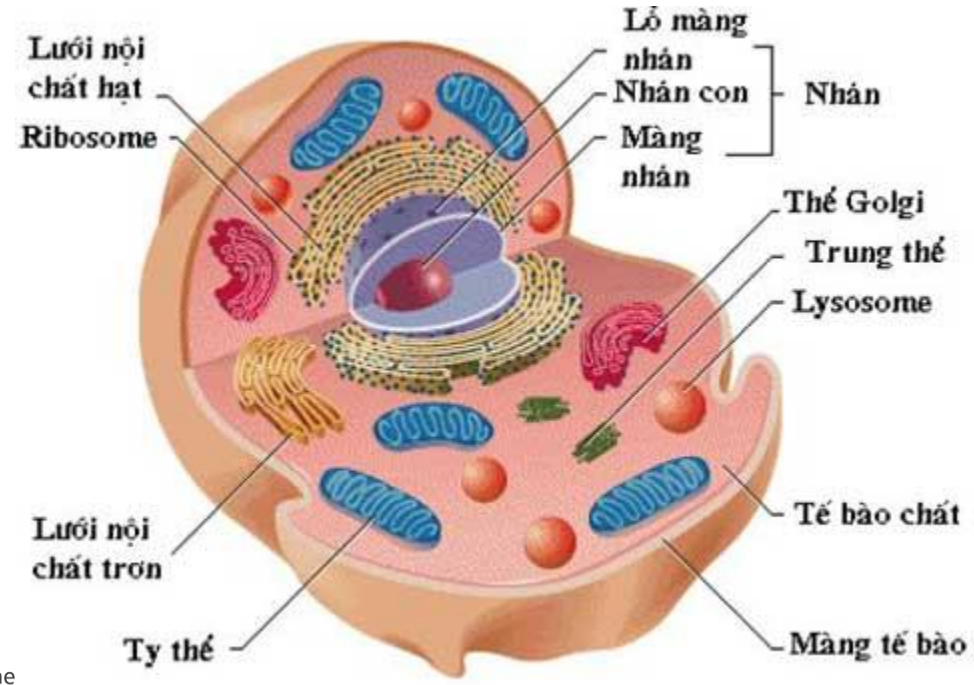
https://mpsuno.vn/insulin-la-gi-insulin-co-vai-tro-nhu-the-nao-doi-voi-con-nguoi/

The role and function of antibodies
Kháng thể



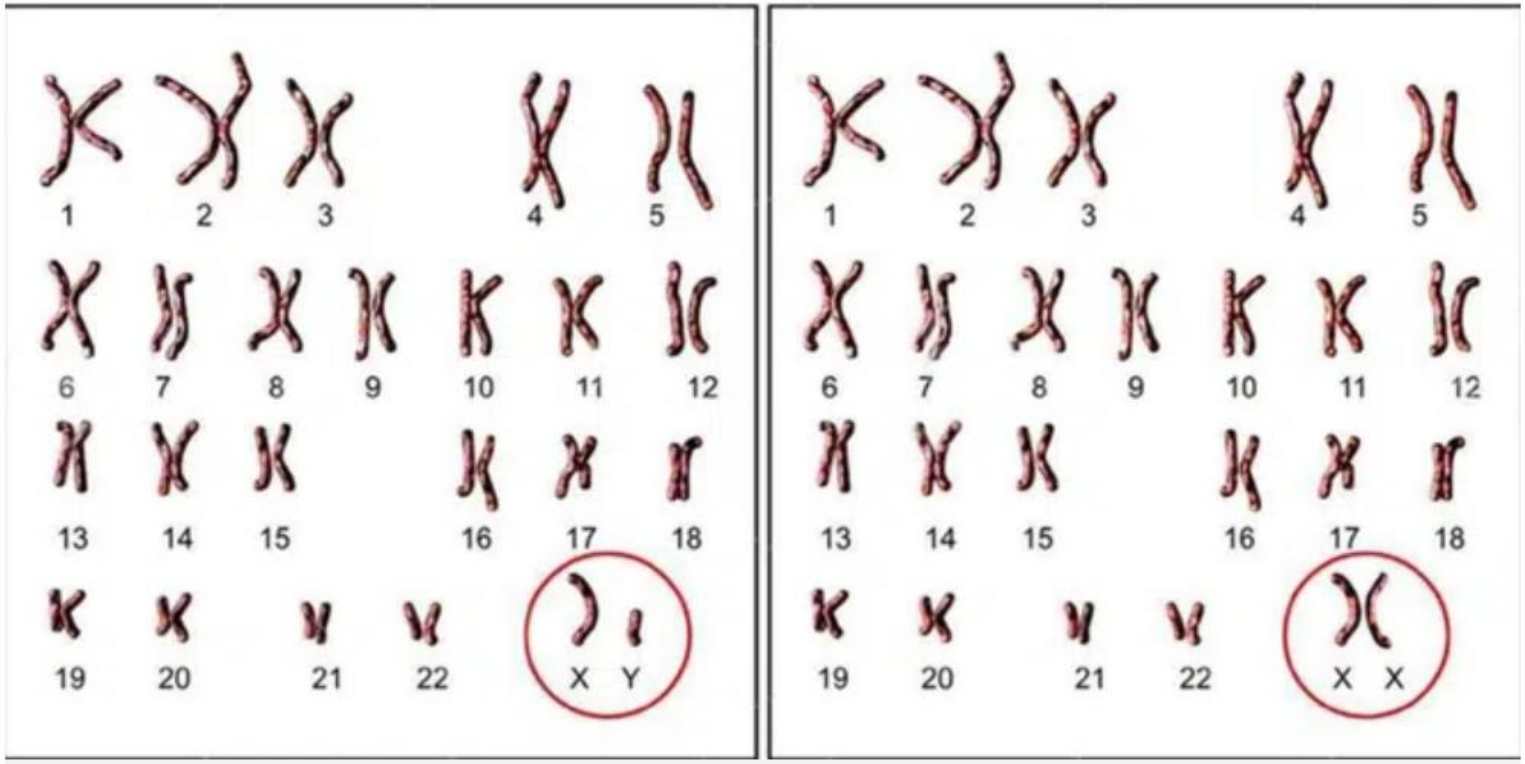
Cell structure





An average person is estimated to contain roughly 30 trillion human cells

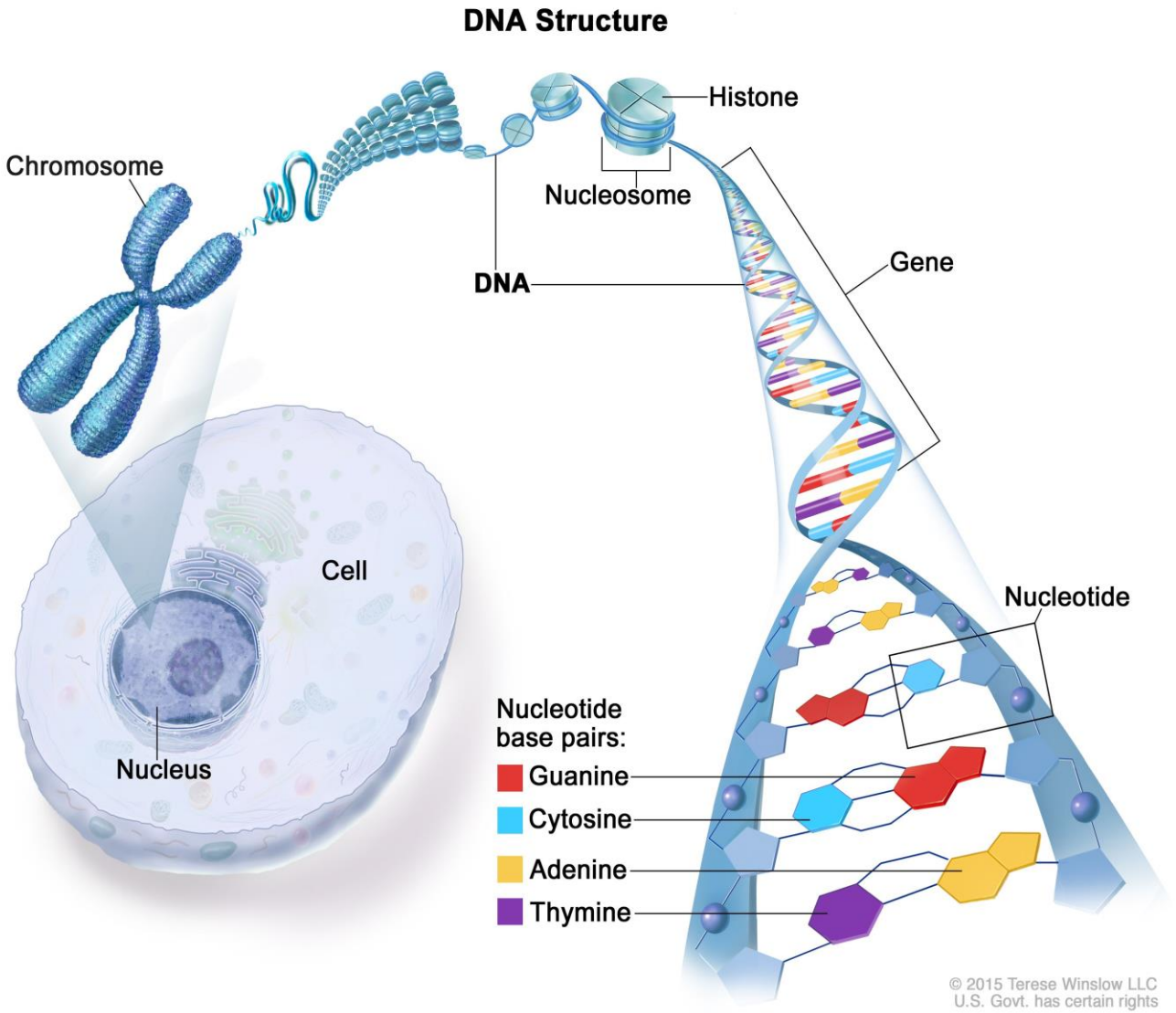
Chromosome and DNA



- Human cells contain 23 pairs of chromosomes.
- We inherit half of our DNA from our fathers and half from our mothers.

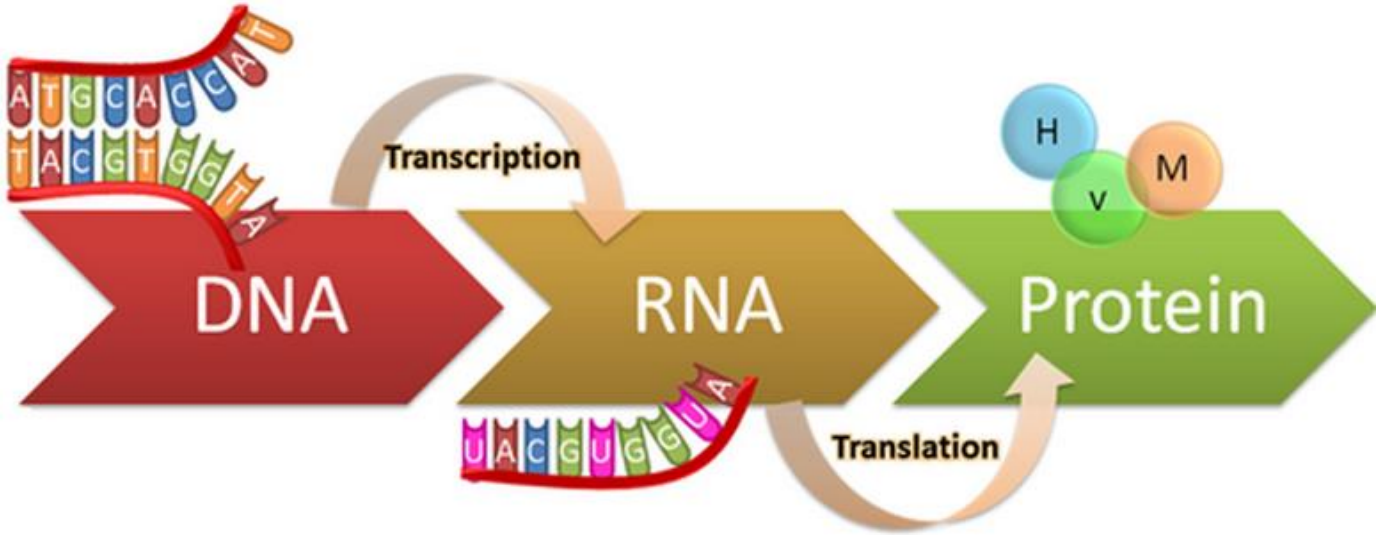
Deoxyribonucleic Acid (DNA)

- A complete set of DNA contains 3 billion bases, 20,000 genes, and 23 pairs of chromosomes.
- Gene is a piece of DNA that encodes a protein.
- Estimated average length of a gene: 1000-2000 bp

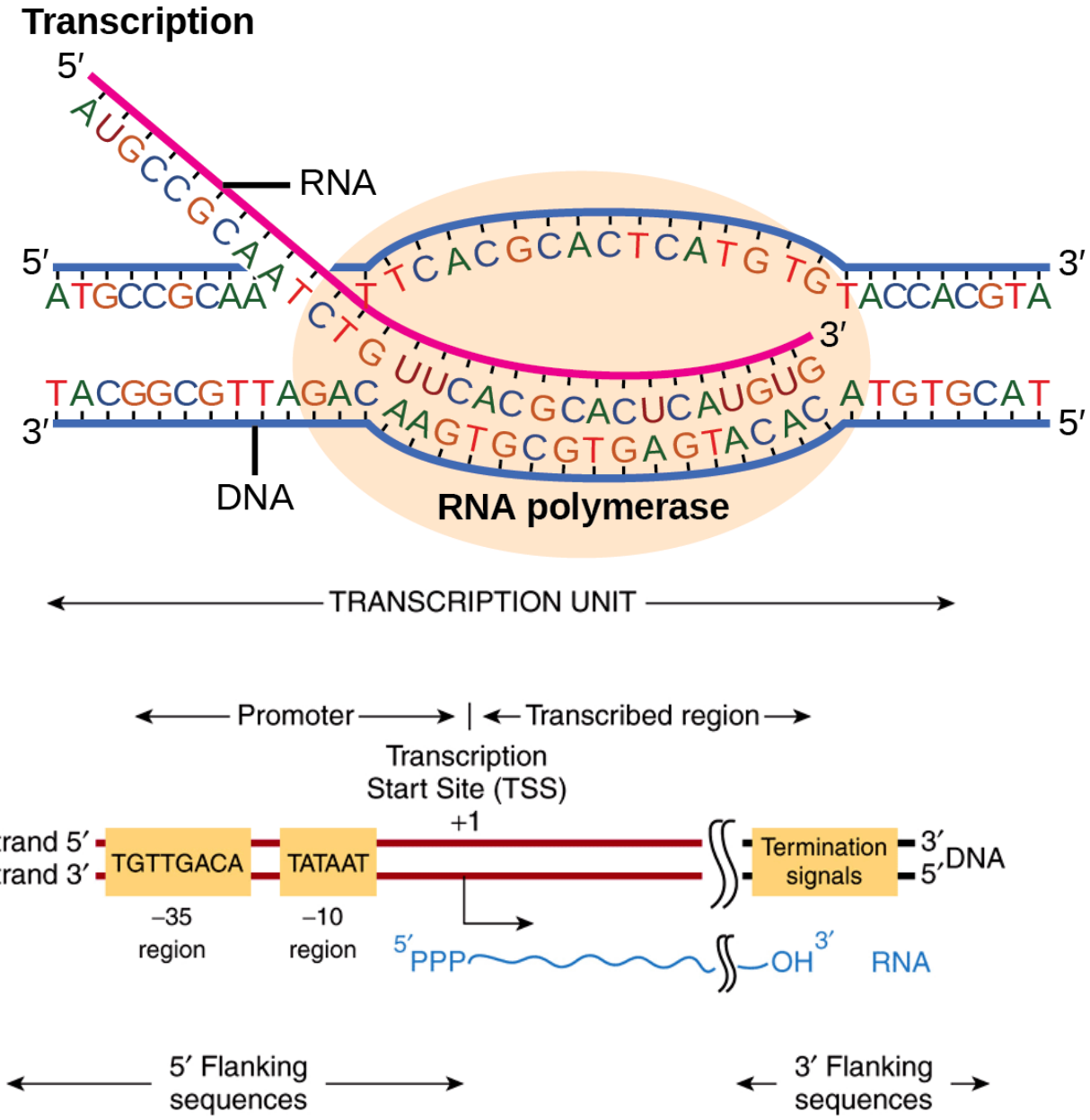


Central Dogma
Học thuyết trung tâm

Francis Crick, James Watson
1962 Nobel Prize for
Physiology or Medicine

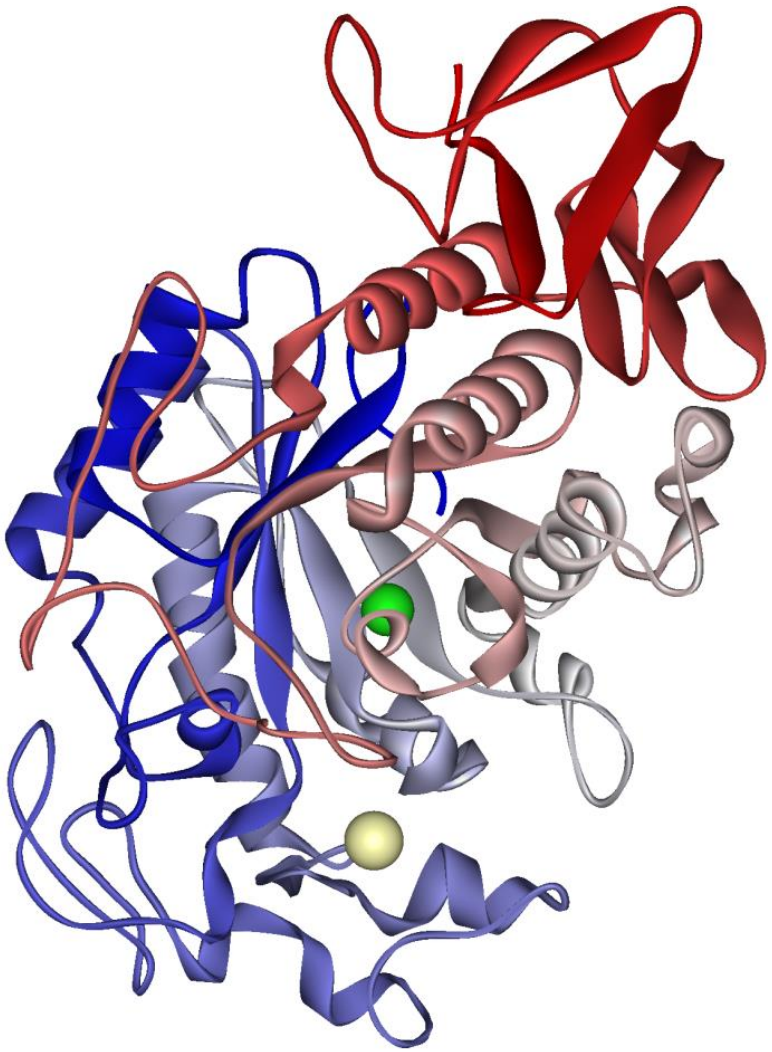


Transcription
Quá trình phiên mã

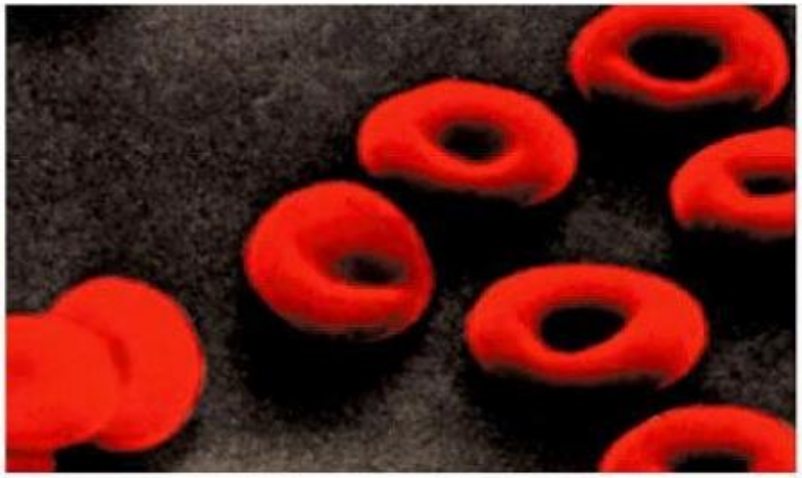


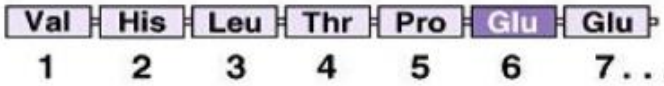
Cấu tạo protein

- Protein is a chain made up of 20 amino acids.
- The length ranges from 20 to more than 5000 amino acids.
- On average, protein contains about 350 amino acids.
- Proteins fold into three-dimensional shapes, form blocks, and carry out most of the chemical reactions in the cell.

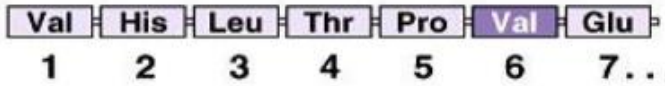


Enzyme Amylase



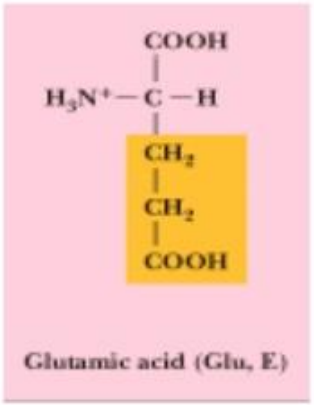


(a) Normal red blood cells and normal hemoglobin

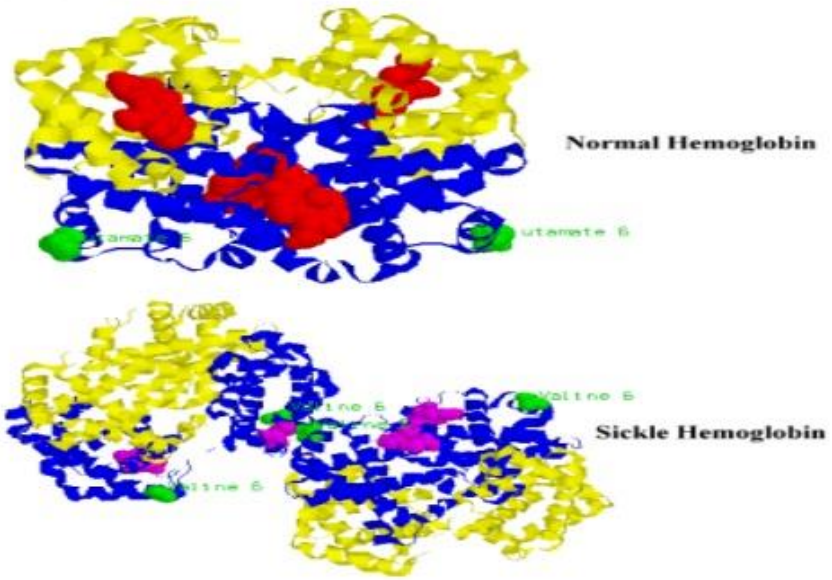


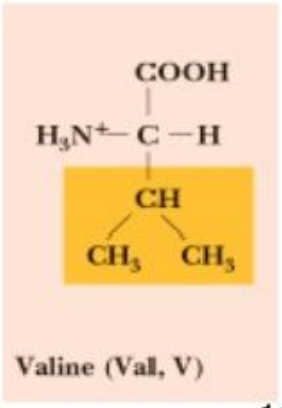
(b) Sickled red blood cells and sickle-cell hemoglobin

Copyright © Pearson Education, Inc., publish



Glutamic acid (Glu, E)

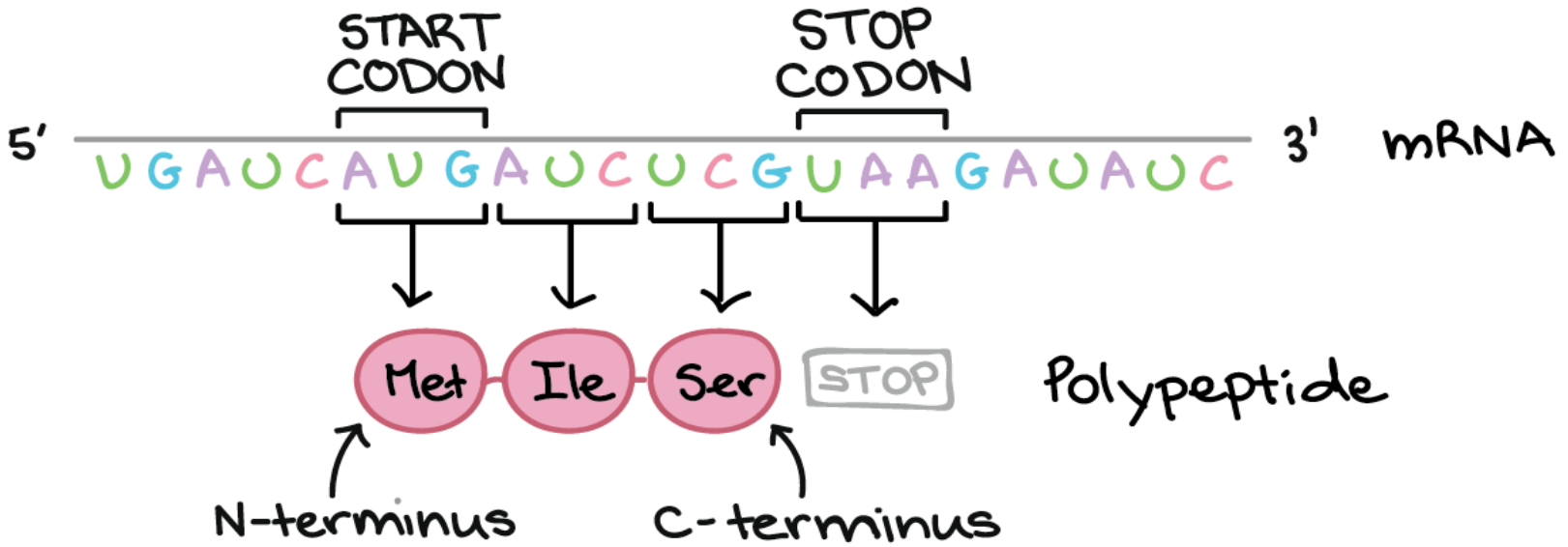


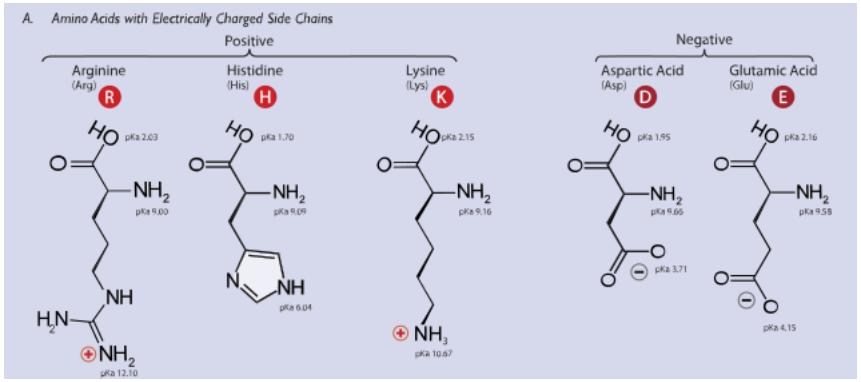


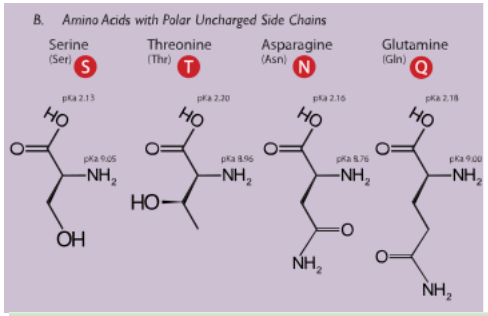
Valine (Val, V)

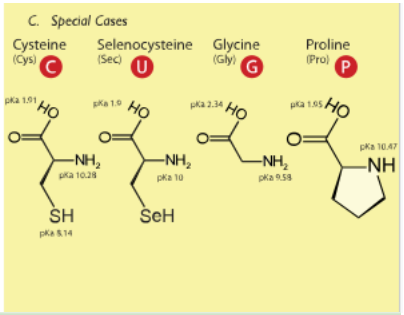
Note: The Sickle hemoglobin image is drawn at 50% of the size of the Normal hemoglobin

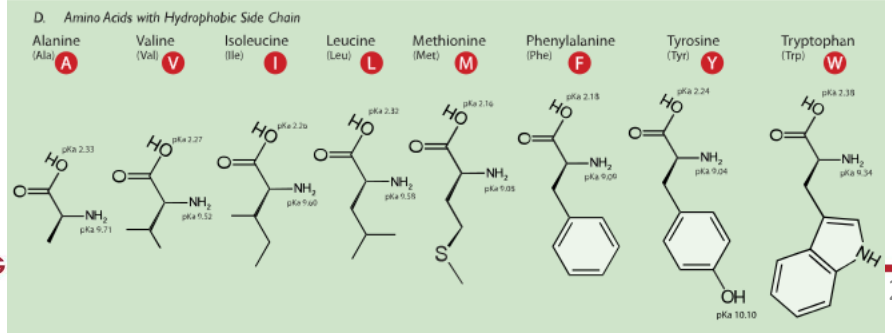
Translation - Quá trình dịch mã



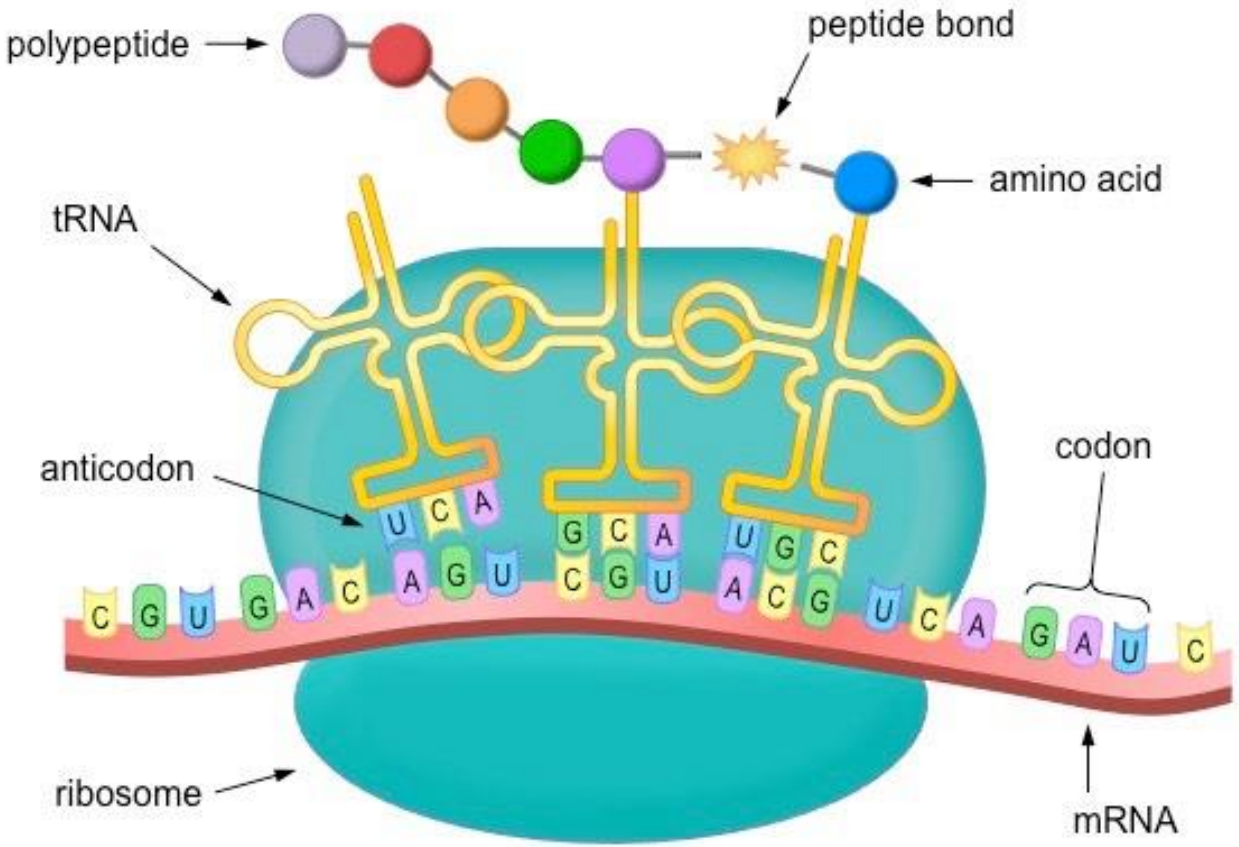




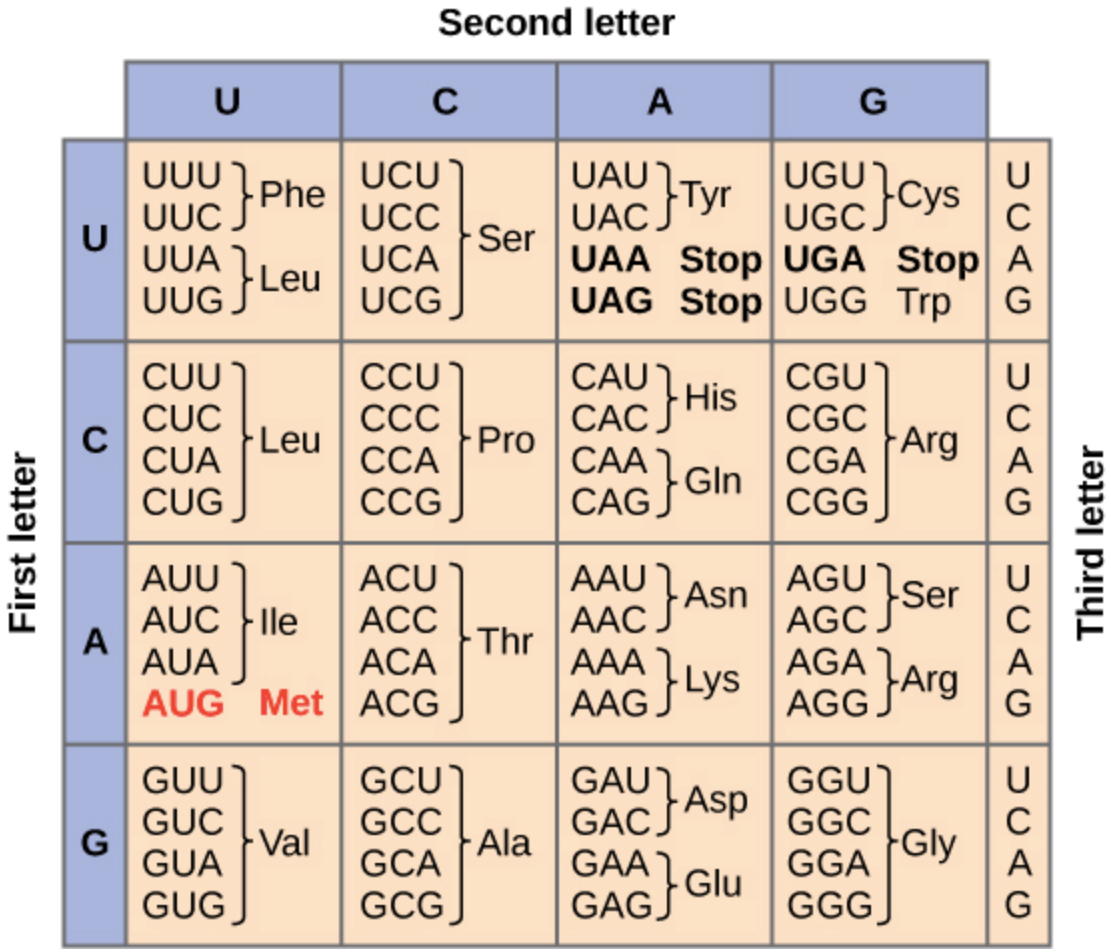




Translation - Quá trình dịch mã

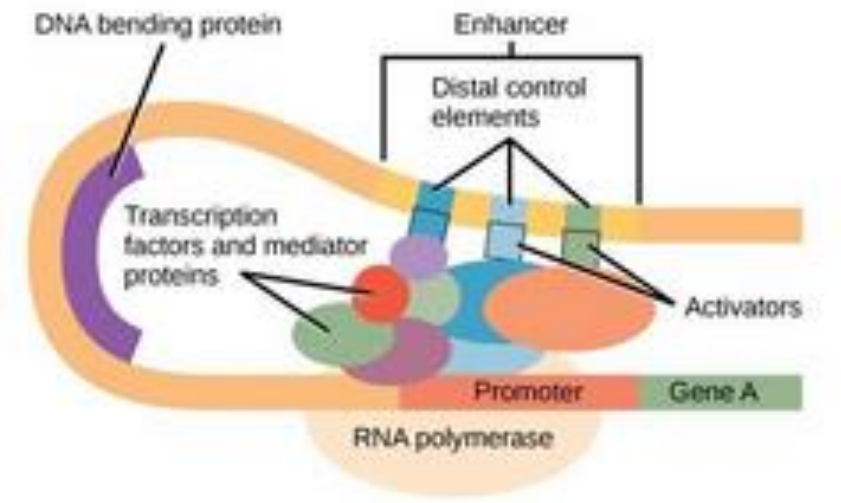


Genetic code – Bảng mã di truyền



The first direction of research
Gene regulation

- Gene regulation is the process of turning genes on and off.



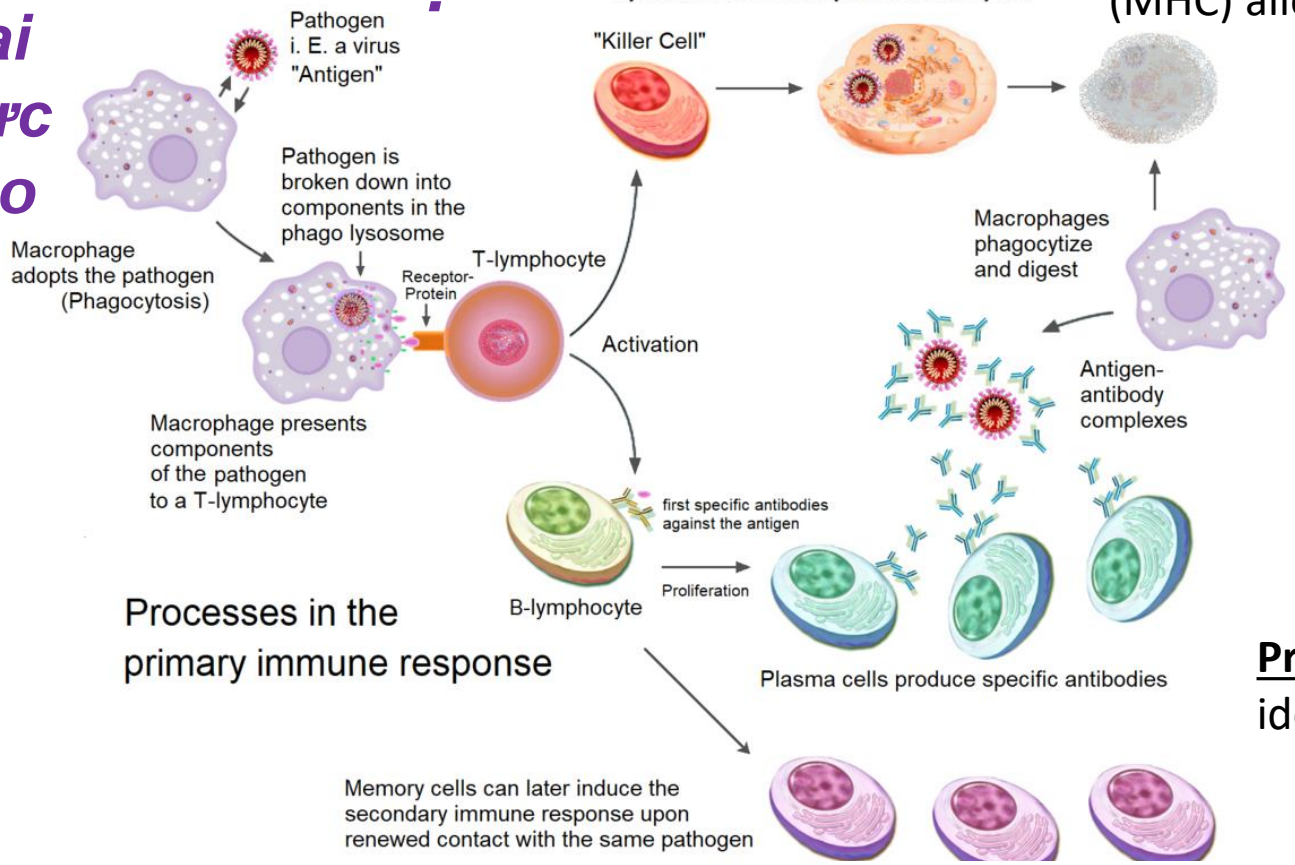
Quang H. Nguyen, Thanh-Hoang Nguyen-Vo, Nguyen Quoc Khanh Le, Trang T.T. Do, Susanto Rahardja, Binh P. Nguyen. iEnhancer-ECNN: identifying enhancers and their strength using ensembles of convolutional neural networks. BMC Genomics 20, 951 (2019), Volume 20 Supplement 9, Published: 24 December 2019

- Regulation of transcription:
  - ***Identifying enhancer regions.***
  - Interaction between enhancer and promoter.
  - Các nhân tố ảnh hưởng đến các tương tác này.
- Regulate the translation process
- Regulate protein activation

The third direction of research
Immune system (hệ miễn dịch)

mầm bệnh

Đại thực bào



Processes in the primary immune response

Problem 1. Accurate prediction of binding between a major histocompatibility complex (MHC) allele and a peptide

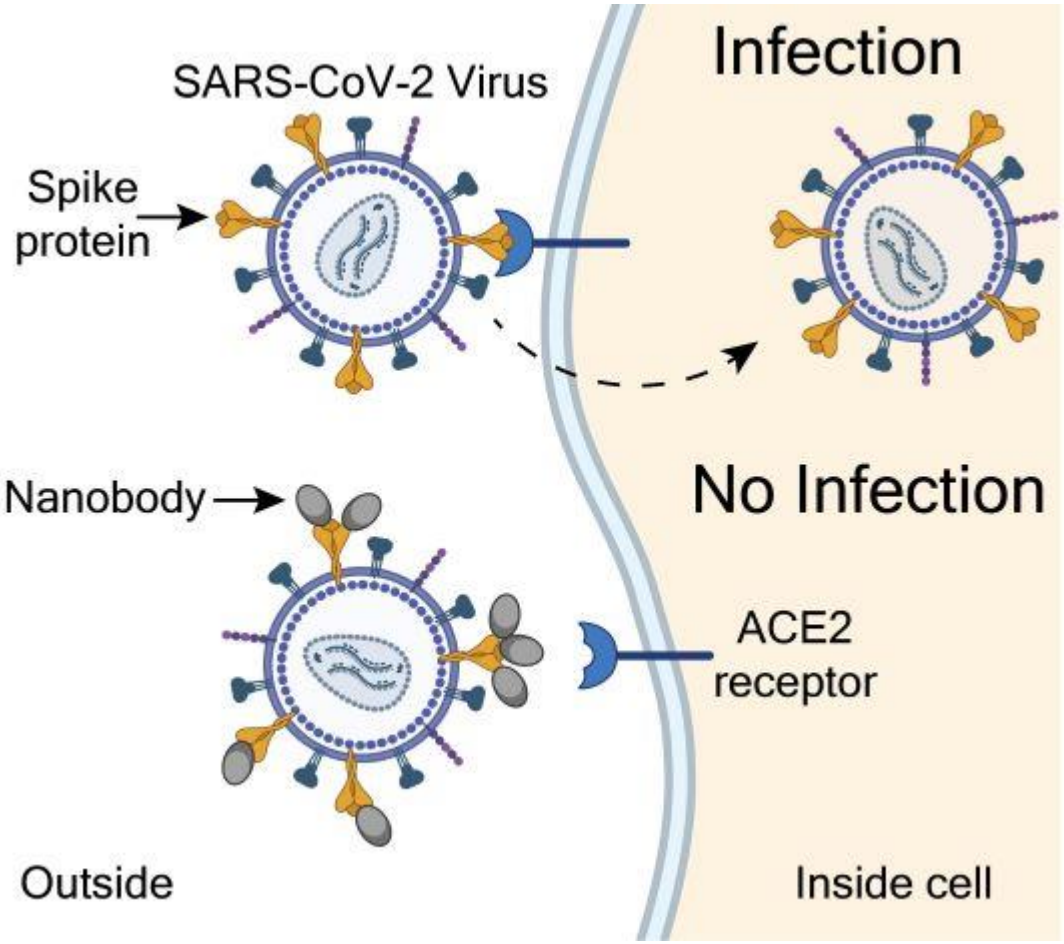
Chế tạo vaccine

Chống virus, Bệnh ung thư

Problem 2. Epitope identification

An **epitope**, also known as **antigenic determinant**, is the part of an antigen that is recognized by the immune system, specifically by antibodies, B cells, or T cells.

The role of antibodies



The third direction of research
Drug discovery

- In the fields of medicine, biotechnology and pharmacology, drug discovery is the process by which new candidate medications are discovered.
- Problem 1. Estimating Minimum Inhibitory Concentrations of Antibiotics towards Klebsiella Pneumoniae
- Problem 2. Dự đoán khả năng ức chế Enzyme họ CYP450
- Problem 3. Identify Antioxidant Proteins
- Problem 4. Predicting evolutionary patterns of corona-viruses and reverse resistance

Estimating Minimum Inhibitory Concentrations (MIC) of Antibiotics towards Klebsiella Pneumoniae

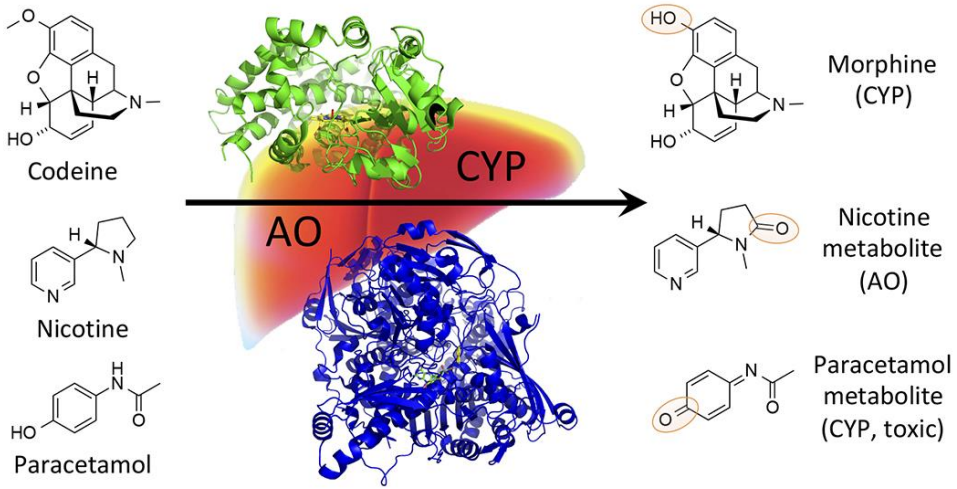
siêu vi khuẩn đa kháng

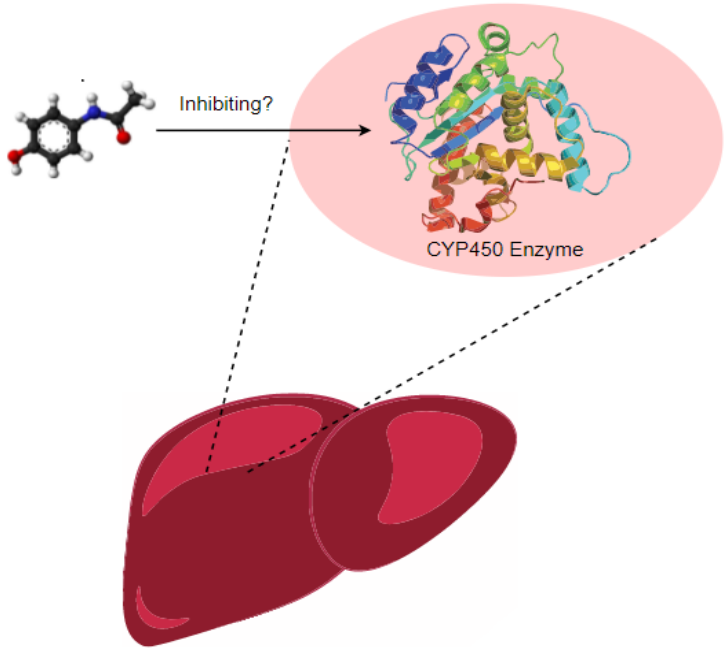
Predict MIC values of 20 antibiotics towards Klebsiella pneumoniae

http://mic.nguyenhongquang.edu.vn/

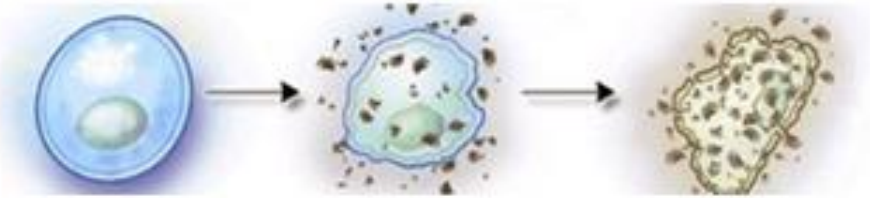
Predicting ability to inhibit CYP450 family enzymes

- Cytochrome P450 (CYP450) enzyme in the liver catalyzes the metabolism of endogenous and exogenous compounds such as drugs, metabolites, or toxins.

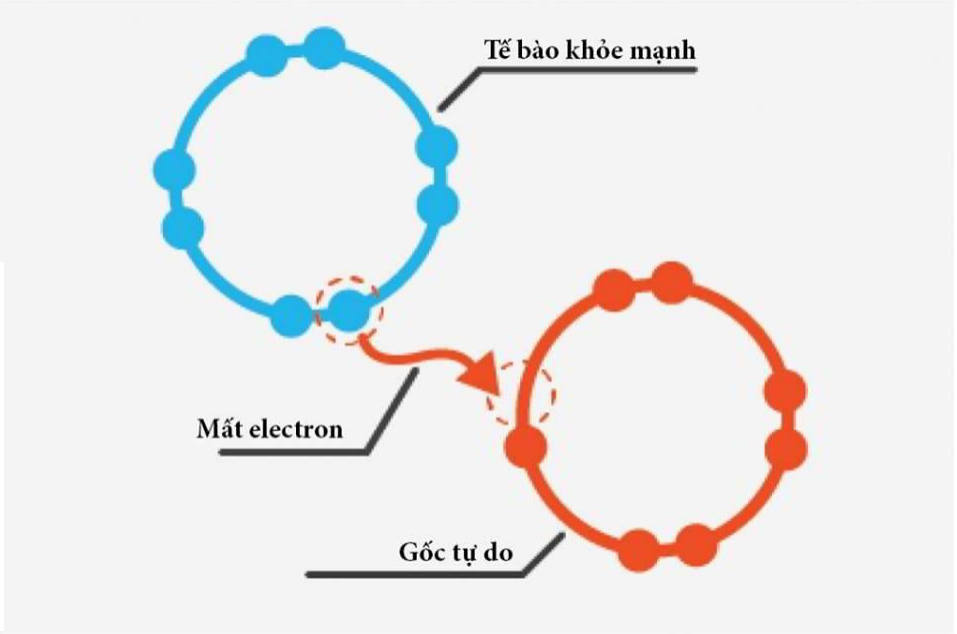


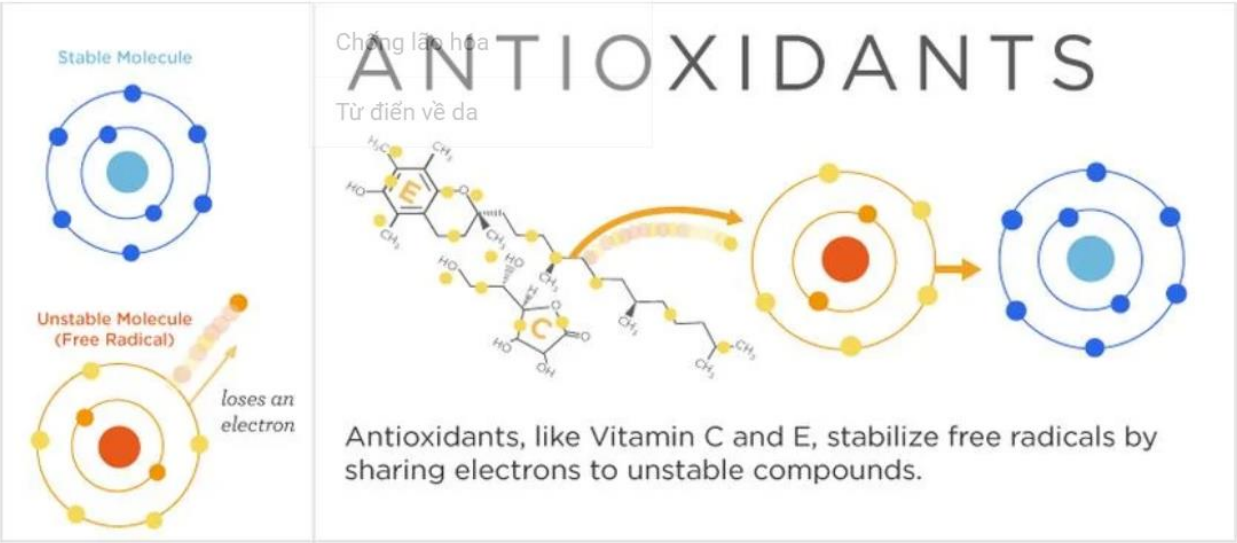


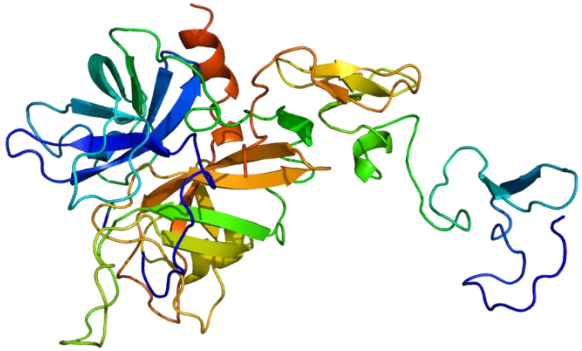
Identify Antixiodant Proteins



Gốc tự do phá hủy tế bào







Antixiodant or not

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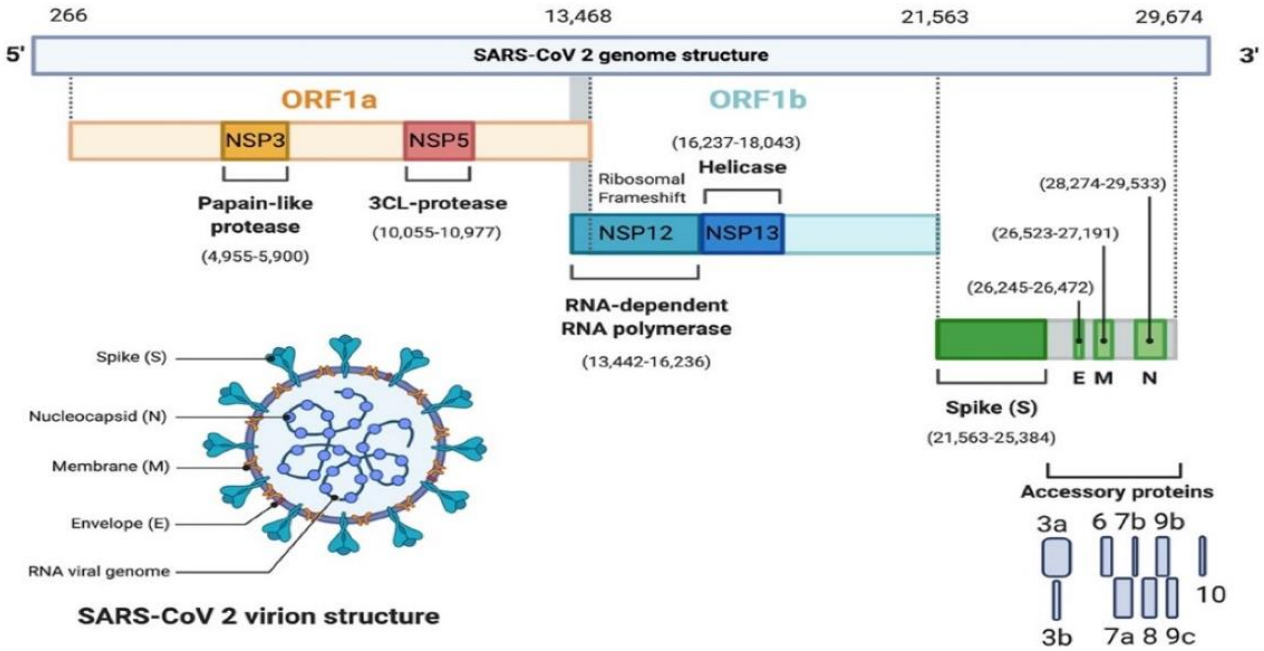
Predicting evolutionary patterns of corona-viruses and reverse resistance



- Learn evolutionary patterns of coronaviruses throughout the time
- Return future mutations
- Predict risks of drug resistance

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References

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