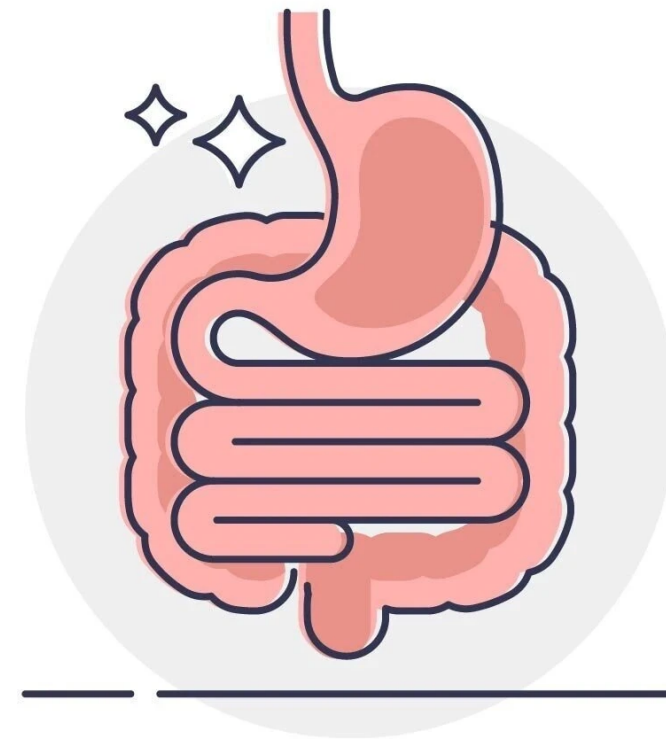


Structural Biology

Ruchika Bajaj, PhD
Membrane Protein Biologist

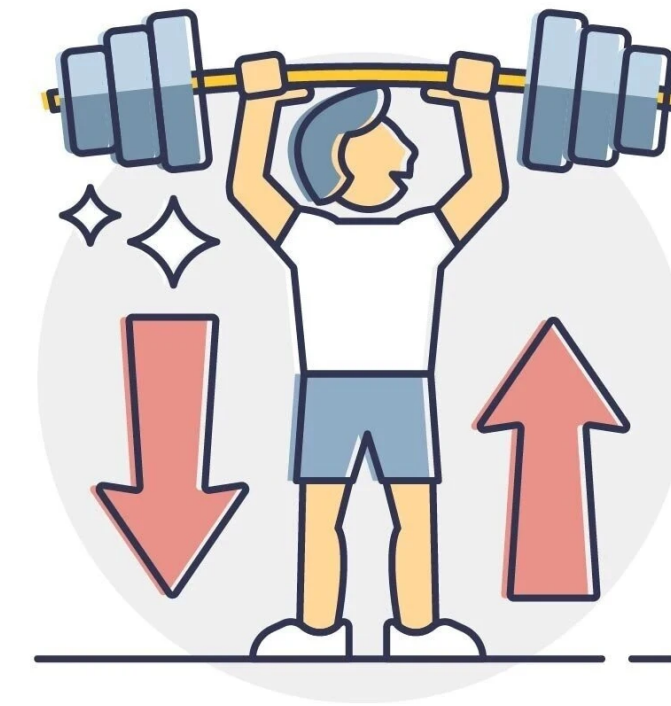
Why do we eat proteins ??



Digestive enzymes help facilitate chemical reactions



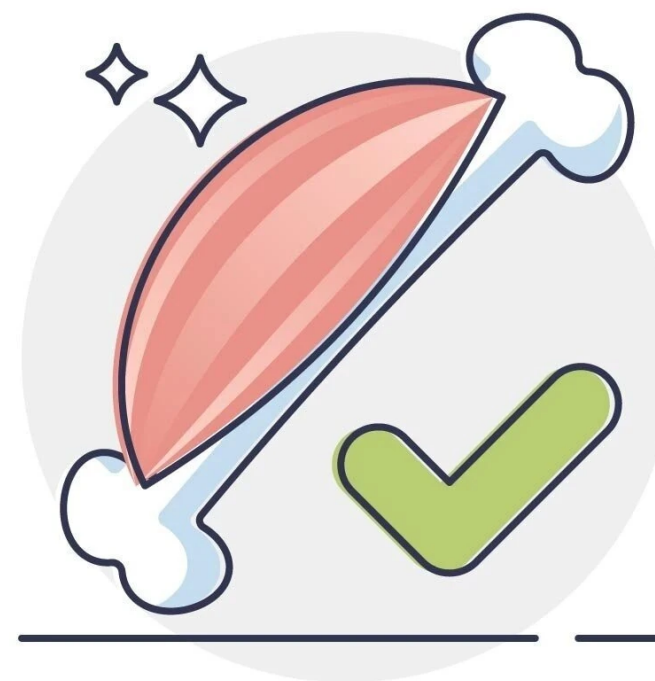
Antibodies support immune function



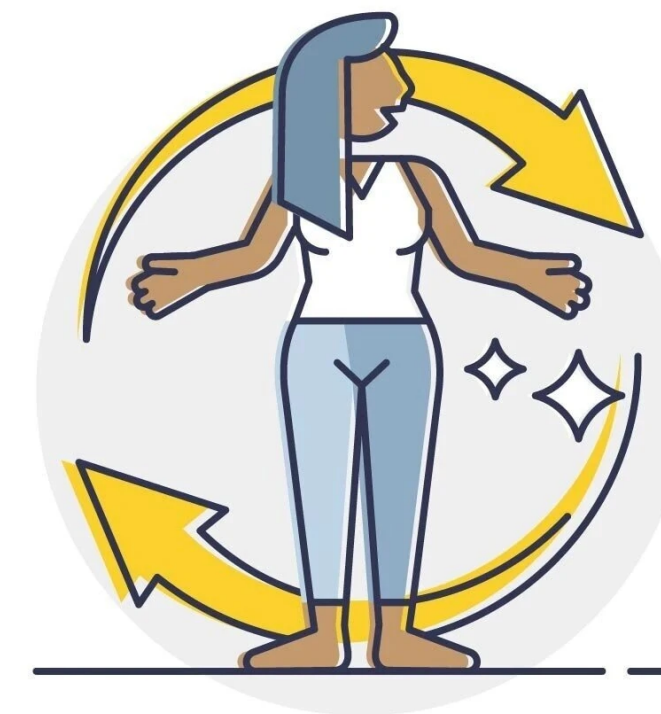
Support muscle contraction and movement



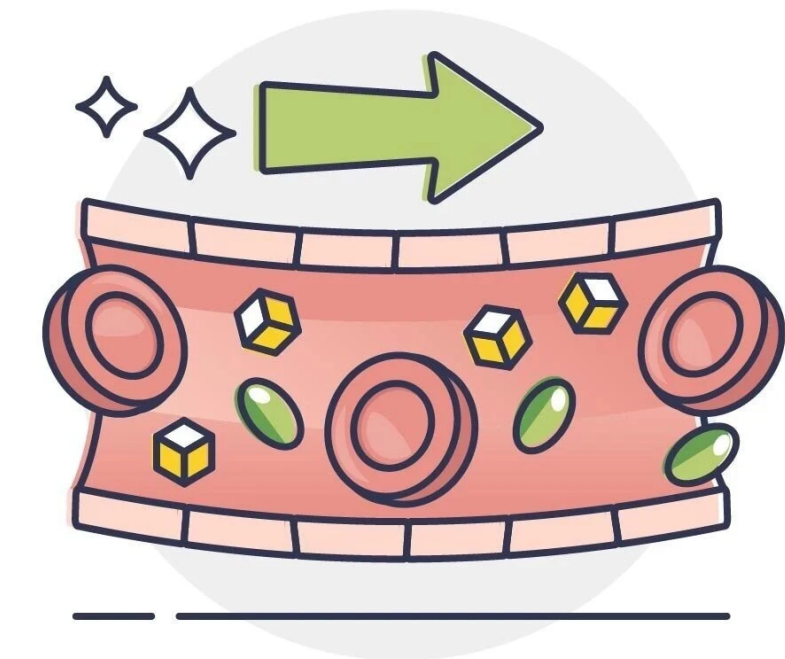
Support the regulation and expression of DNA and RNA



Provide support to the body



Hormones help coordinate bodily function



Move essential molecules around the body

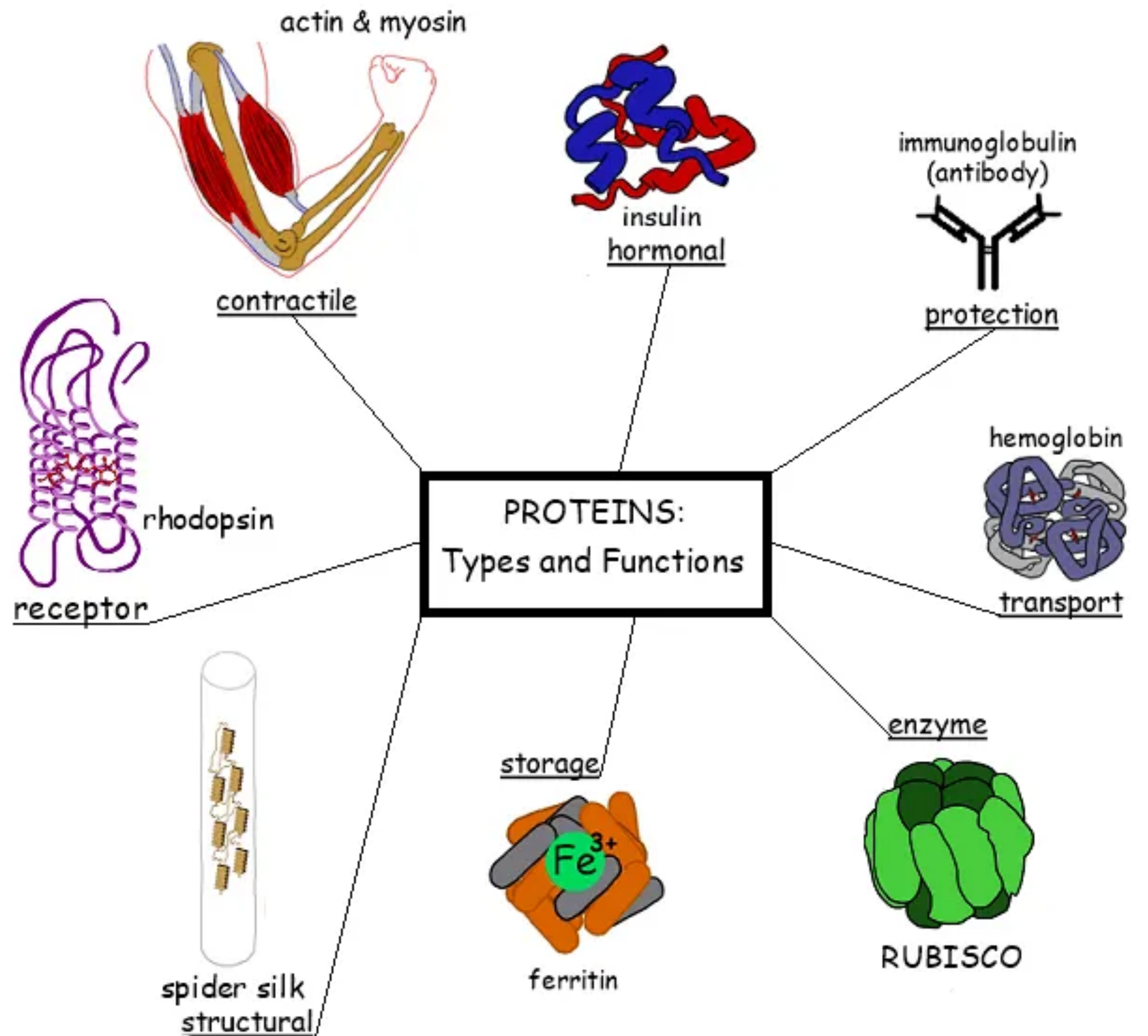
LASCHÉ X[®]

The Importance of Protein in Diet

Why Do We Need **Protein**?

Learn More

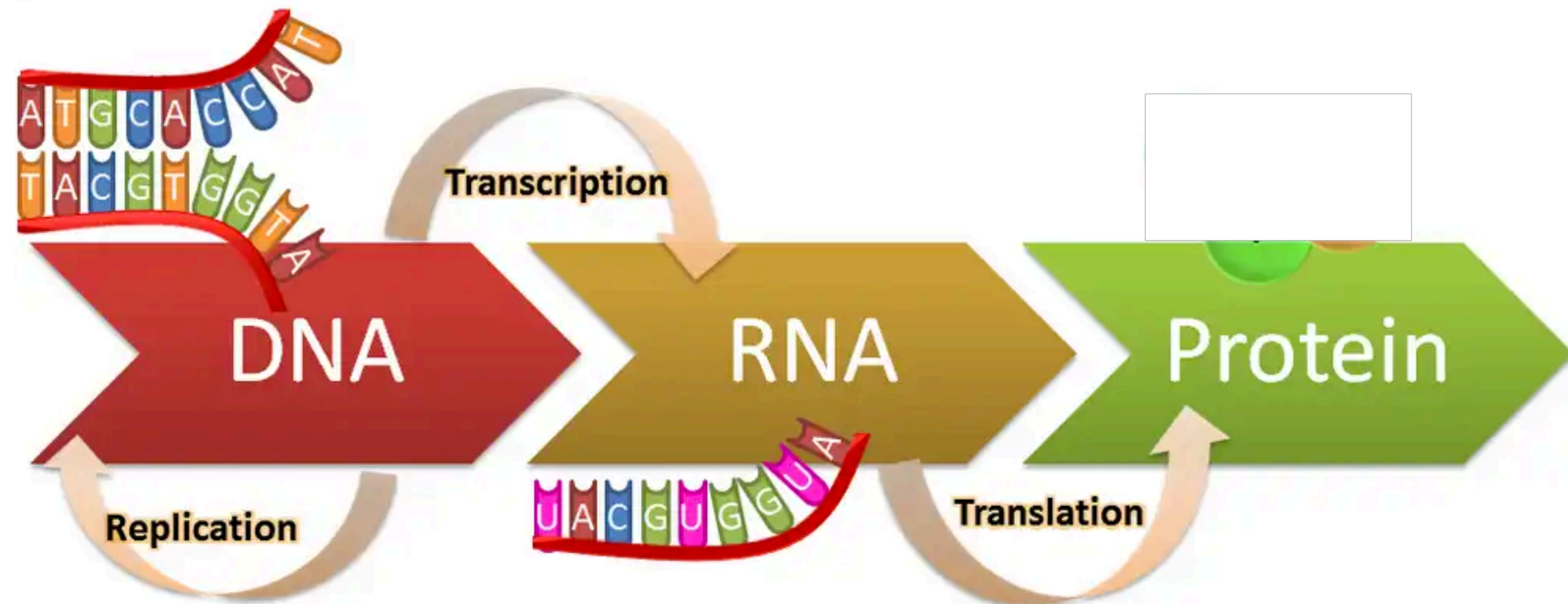
Functions of protein



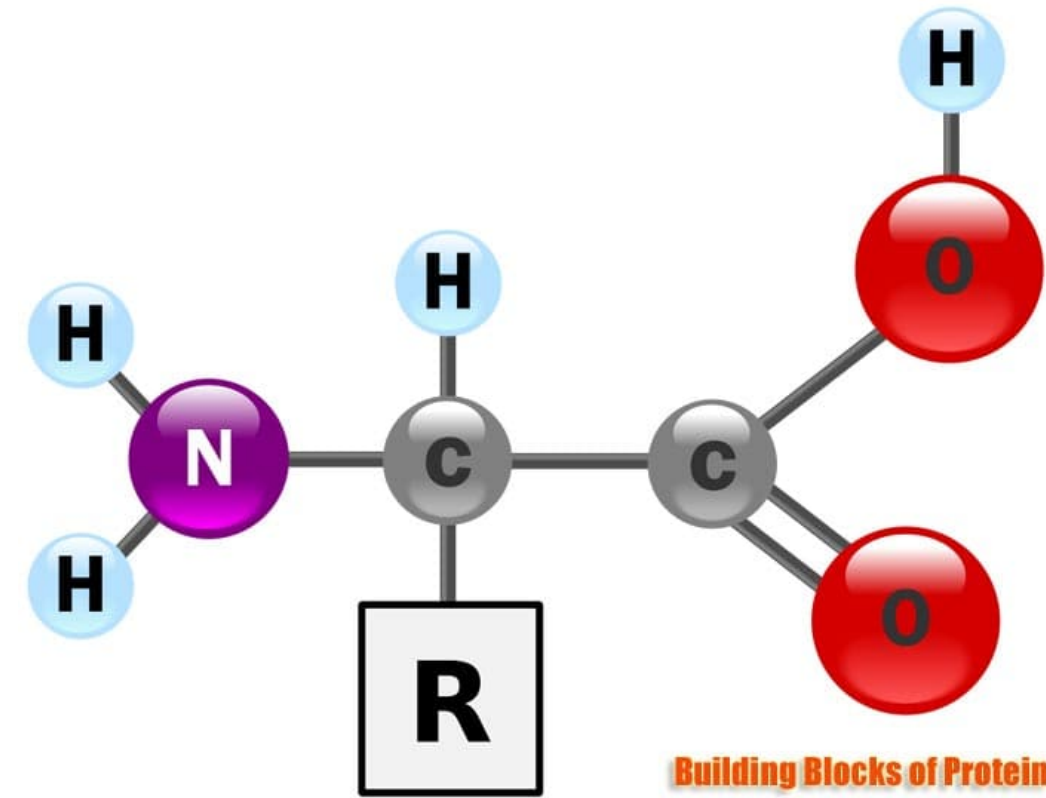
Central Dogma: Proteins : the building block of life



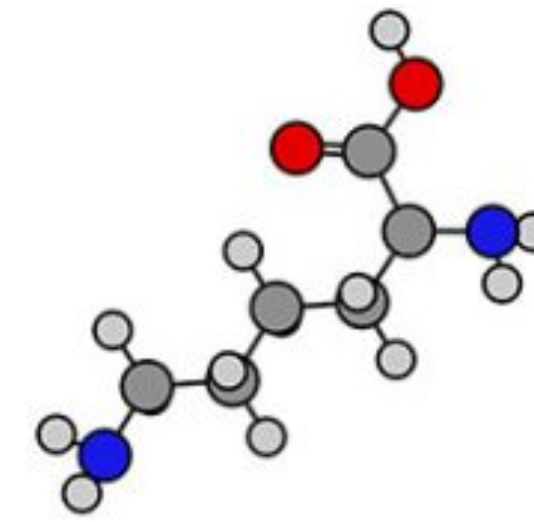
Central Dogma



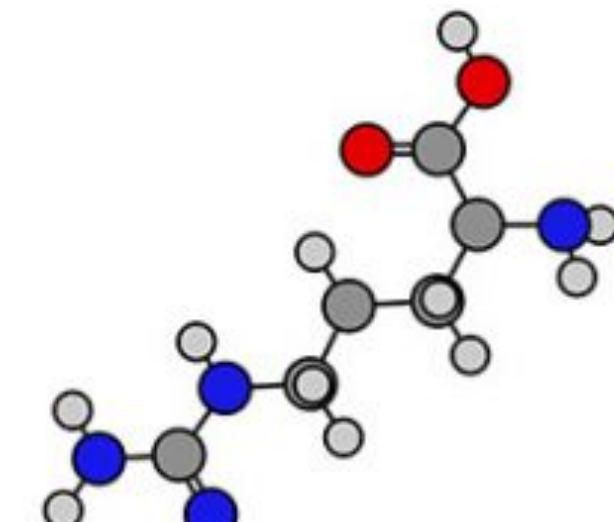
Amino acids : building blocks of proteins



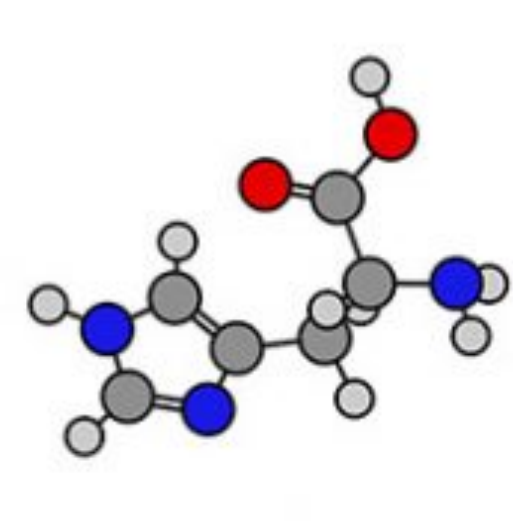
Positively charged



Lysine

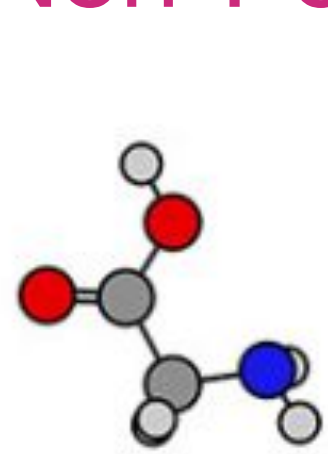


Arginine

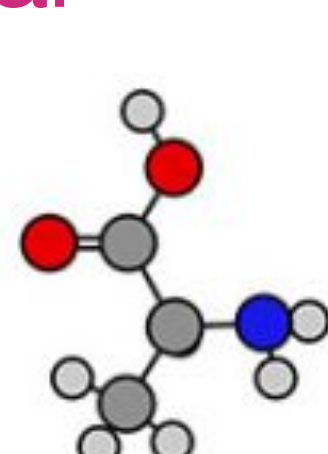


Histidine

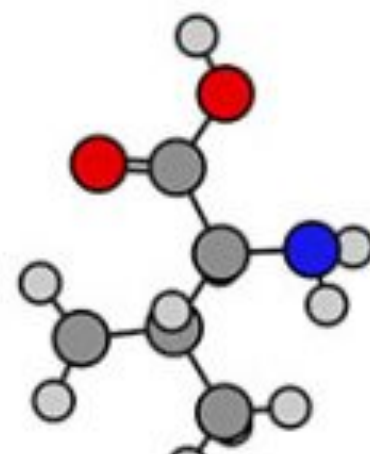
Non-Polar



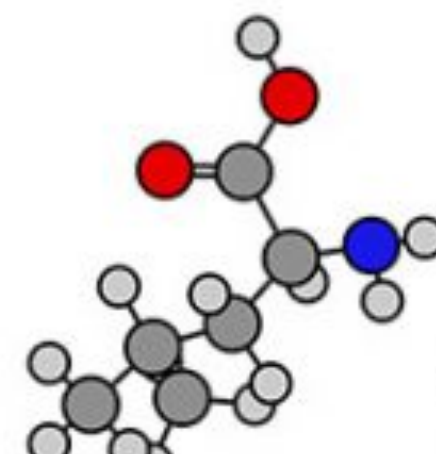
Glycine



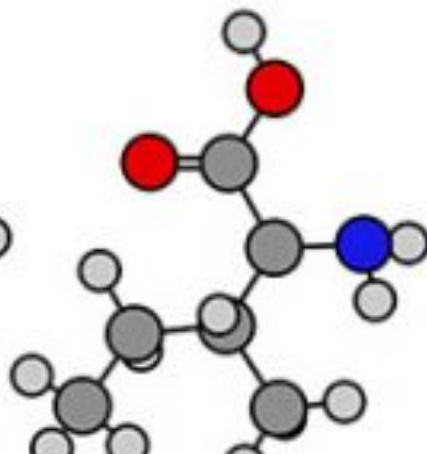
Alanine



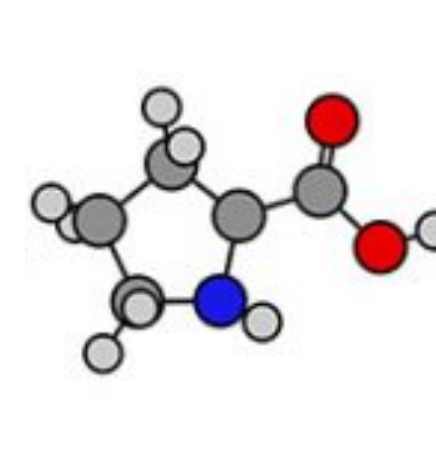
Valine



Leucine

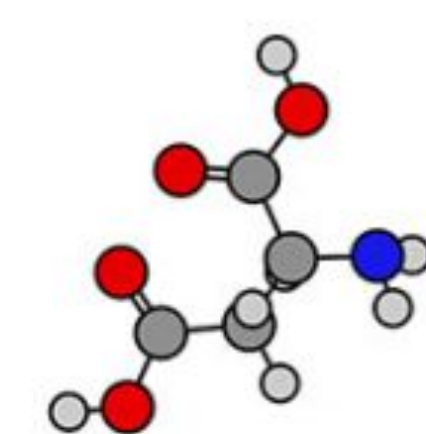


Isoleucine

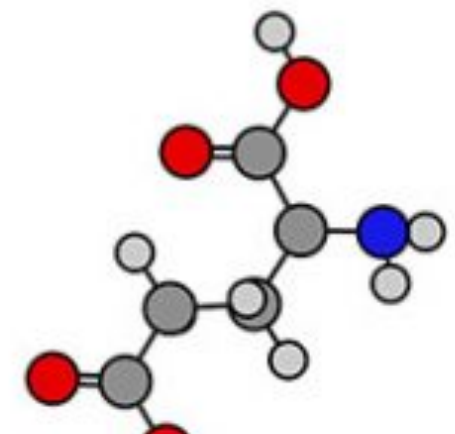


Proline

Negatively charged

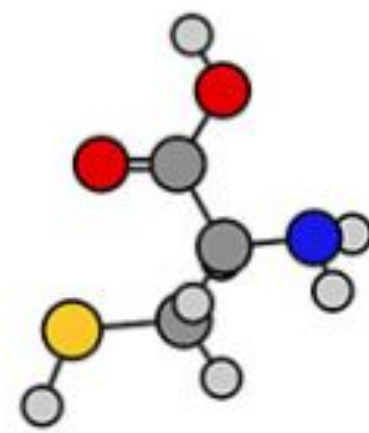


Aspartic acid

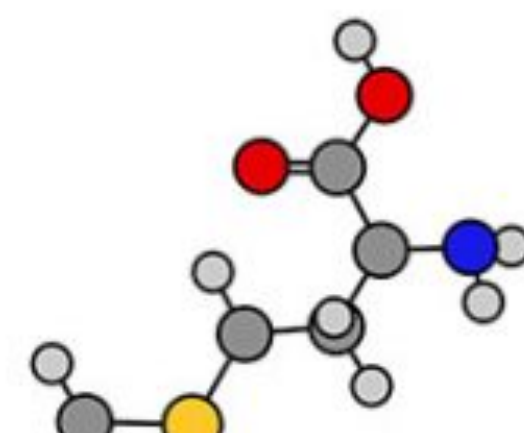


Glutamic acid

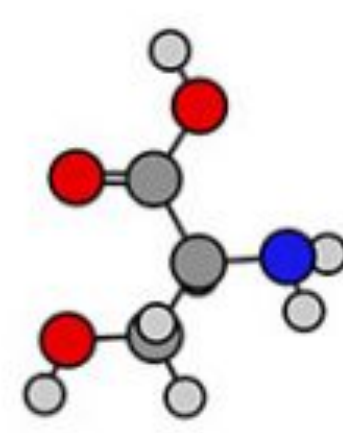
Polar



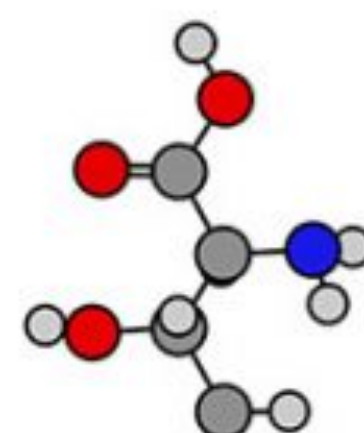
Cysteine



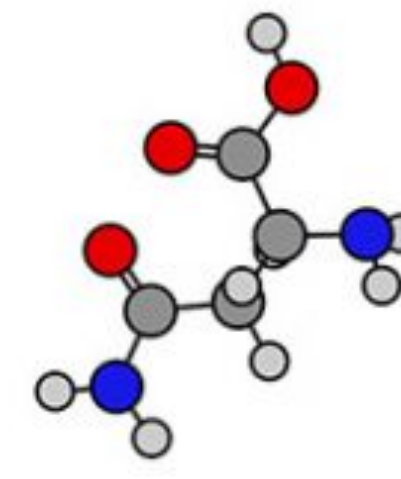
Methionine



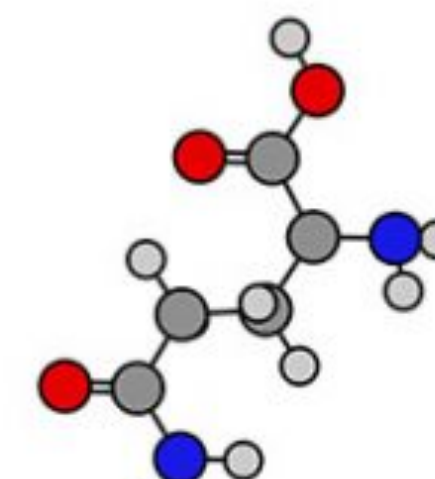
Serine



Threonine

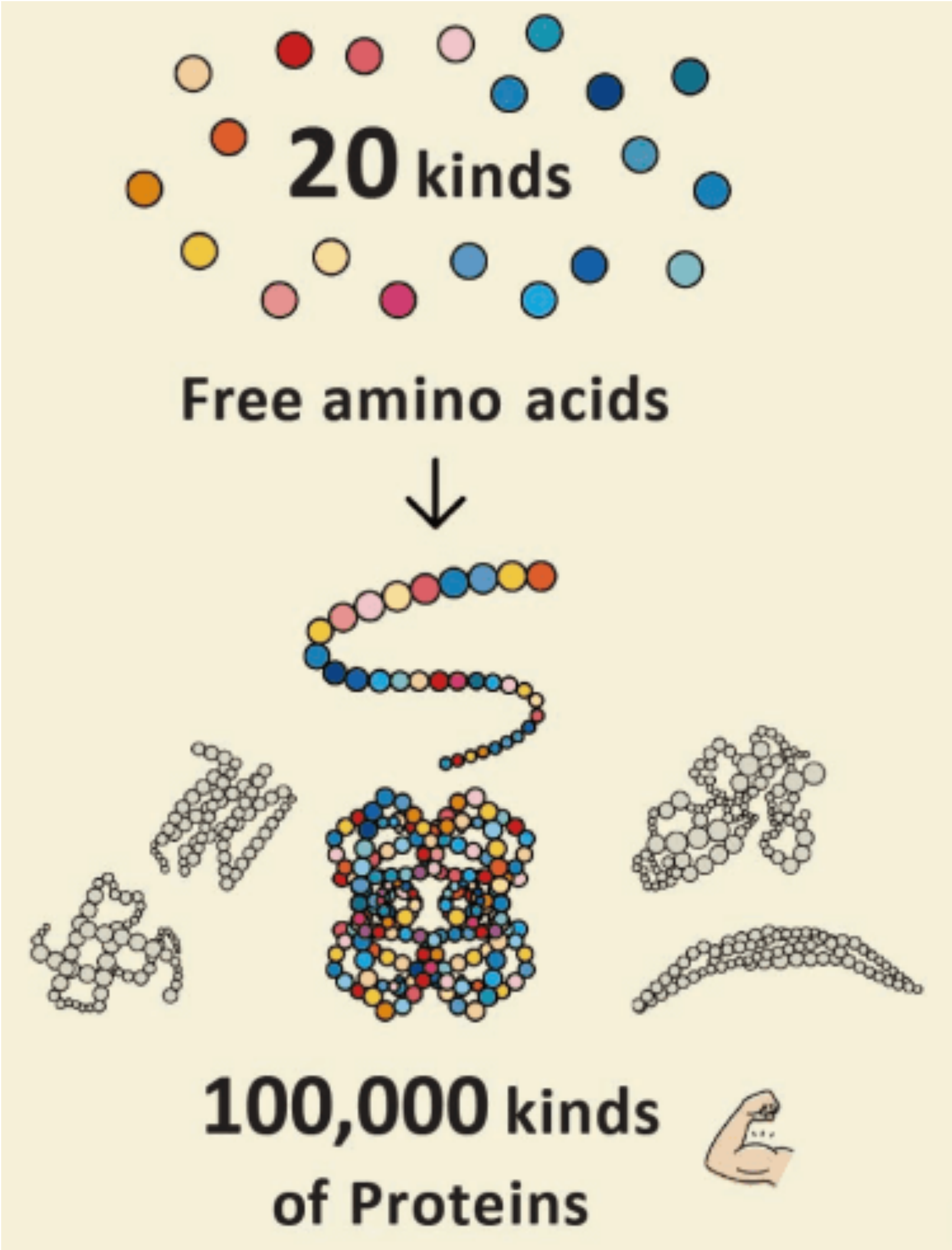
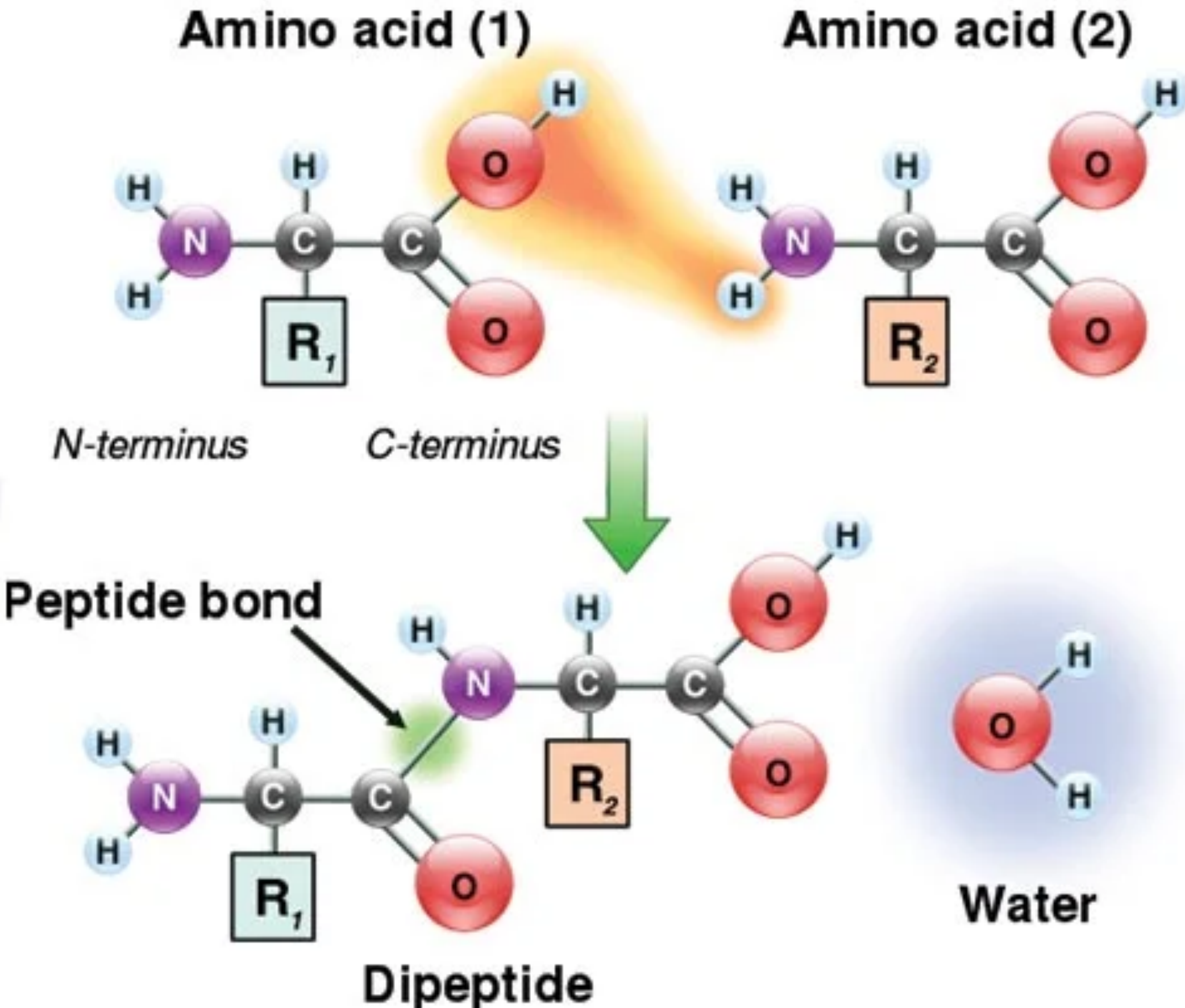


Asparagine

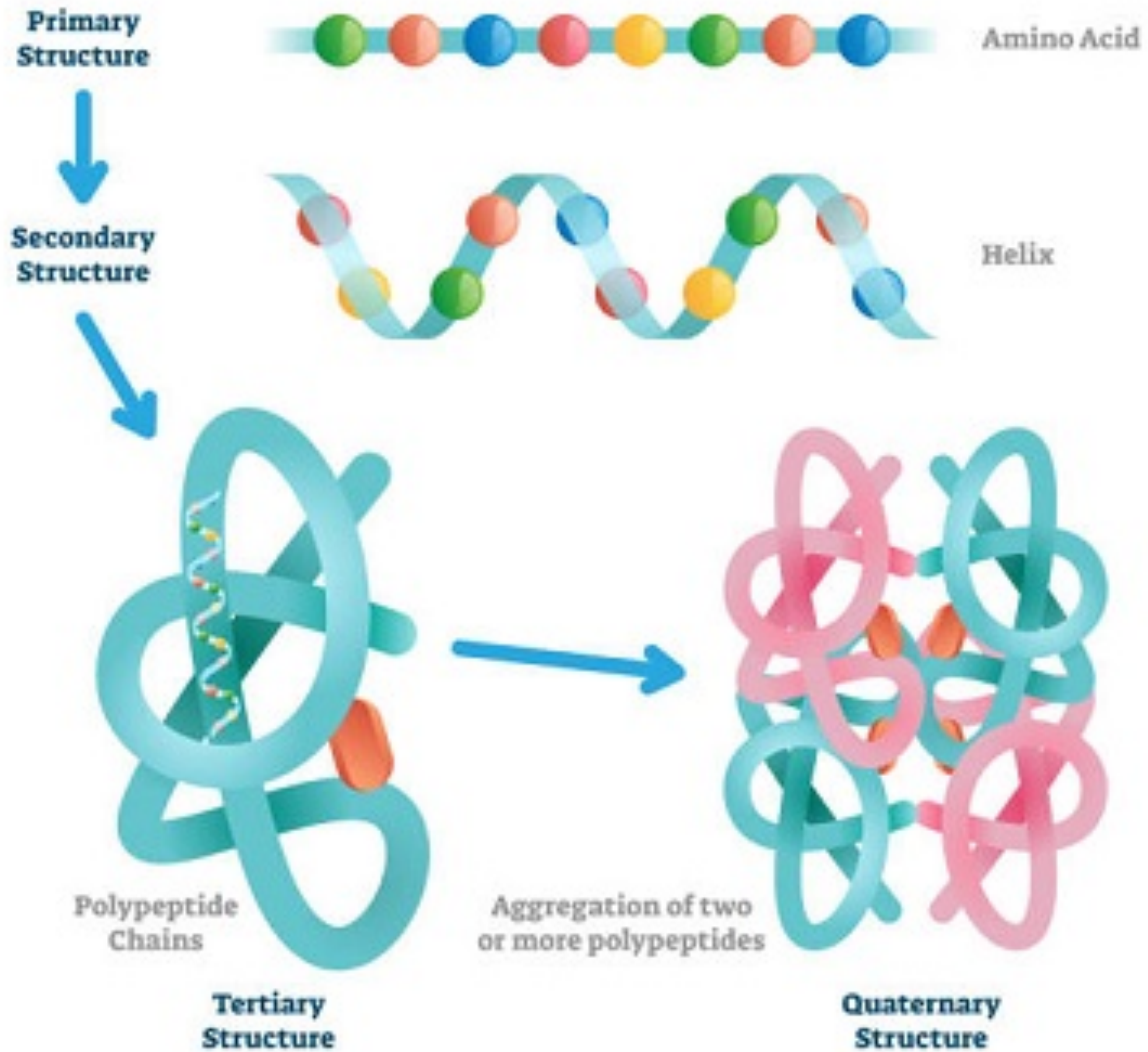


Glutamine

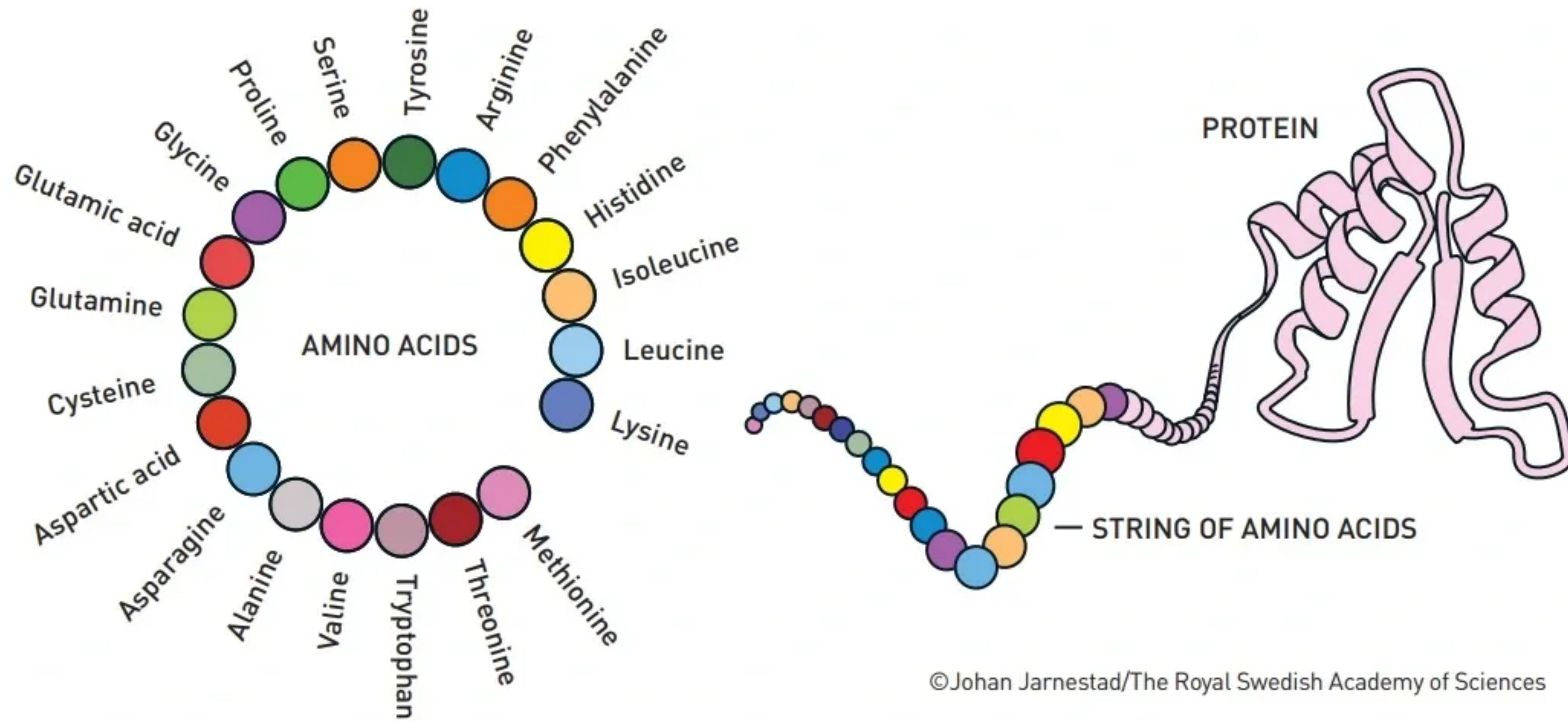
The peptide bond connects amino acids to build peptides



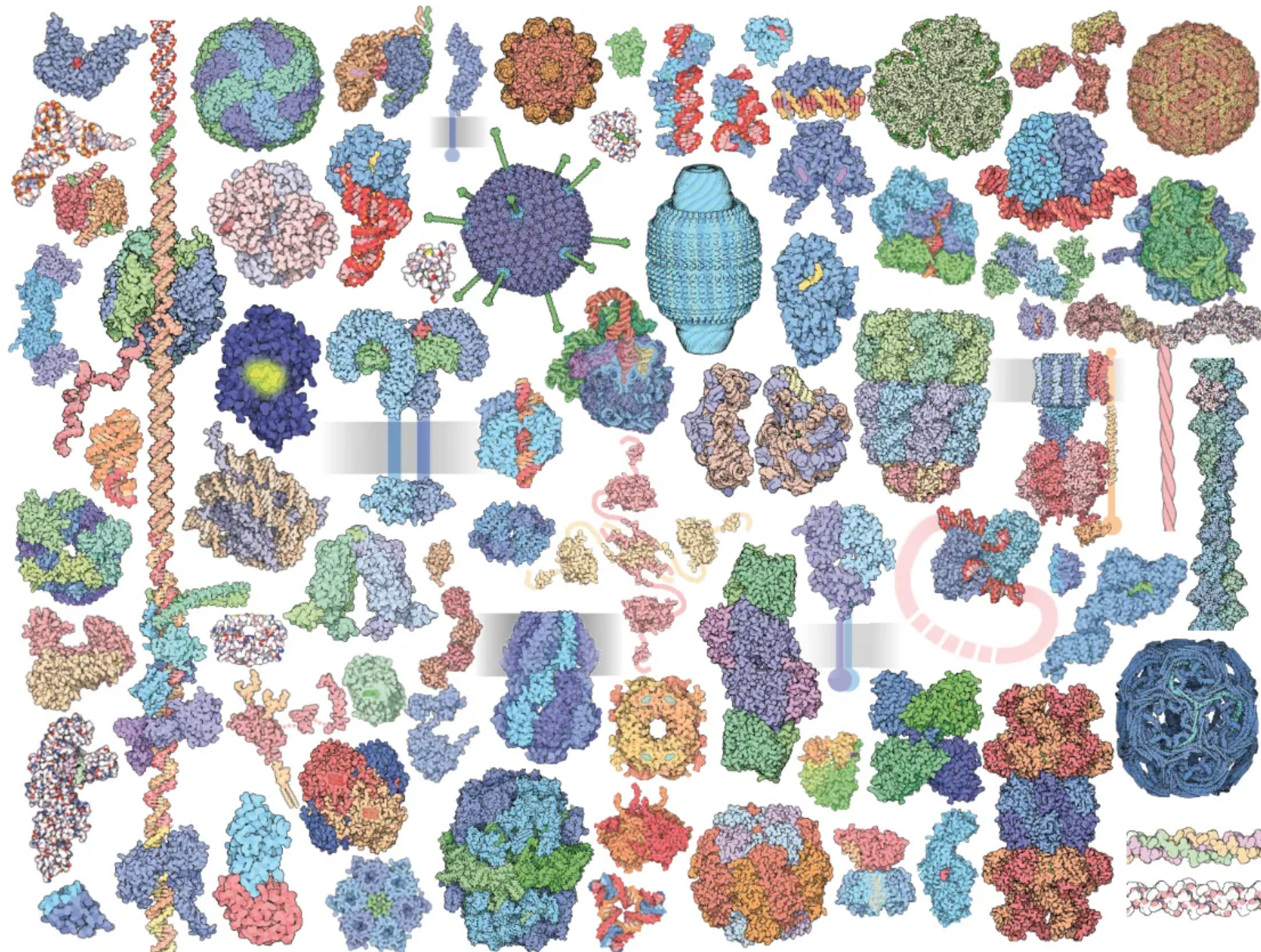
Levels of protein structure



The Folding Problem



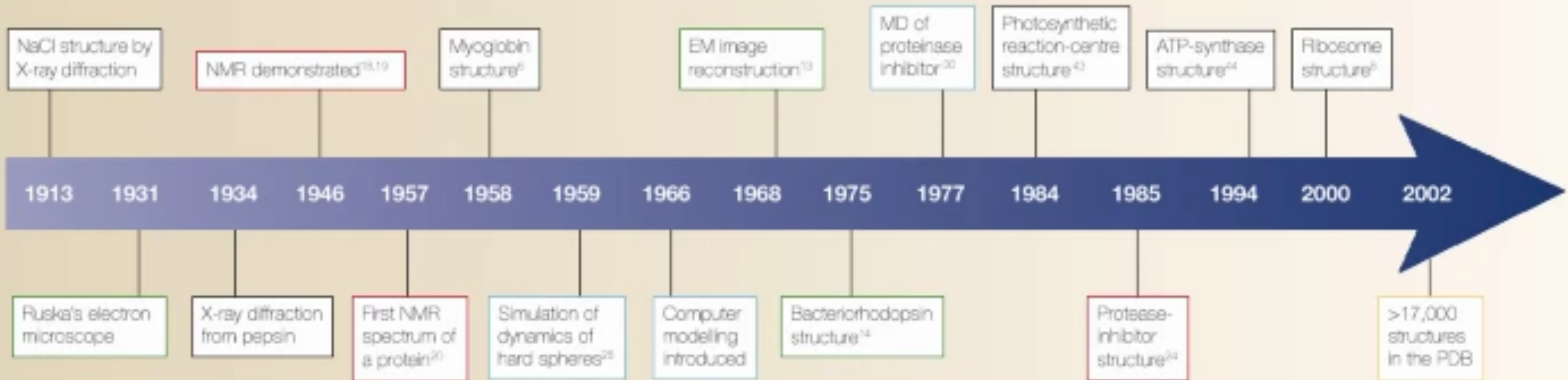
A variety of protein structures



Structural Biology is a mature science

Structural biology is the study of the molecular structure and dynamics of biological macromolecules, particularly proteins and nucleic acids, and how alterations in their structures affect their function. Structural biology incorporates the principles of molecular biology, biochemistry and biophysics.

Timeline | **The march of structural biology**

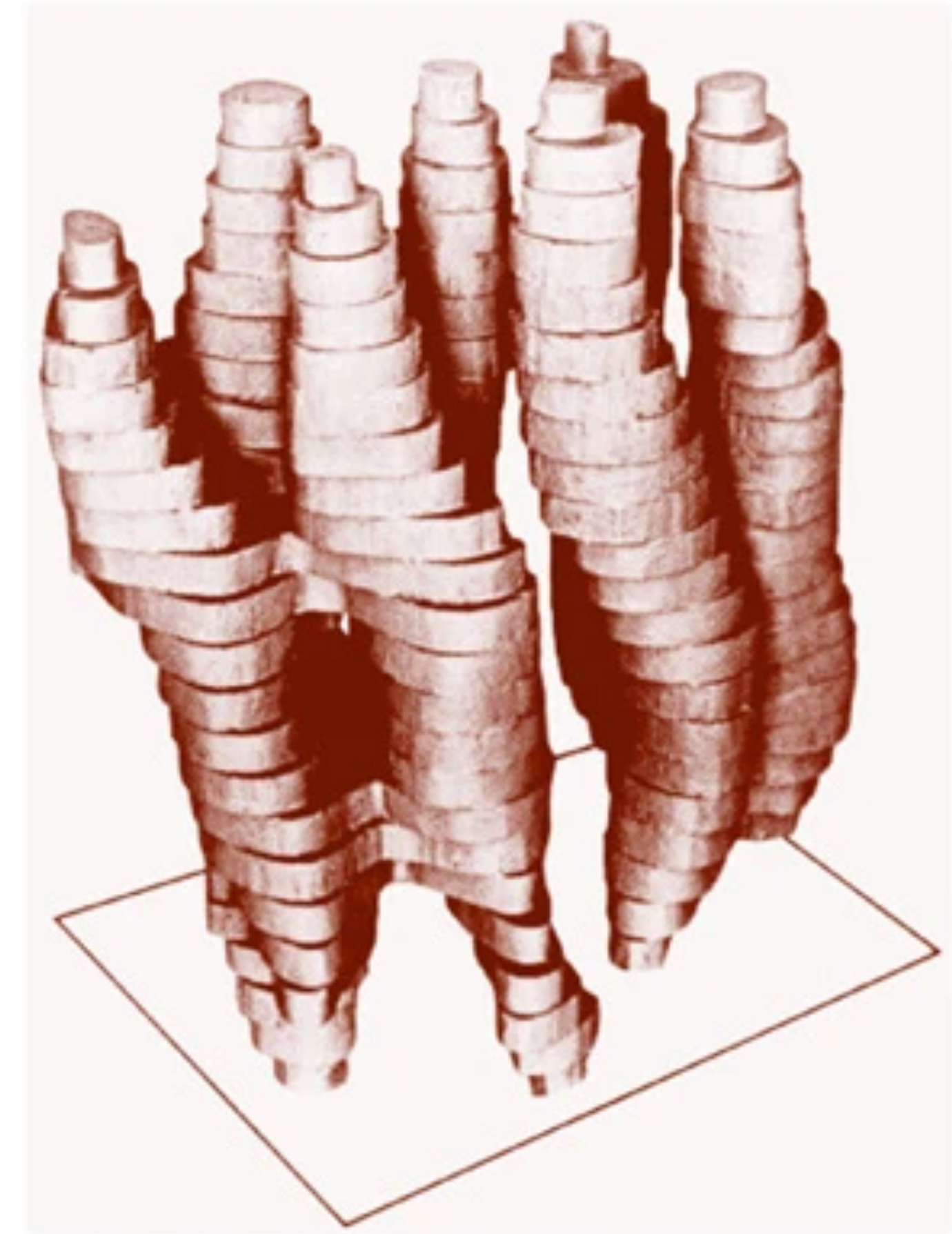


Some of the key developments in crystallography (shown in black), electron microscopy (EM; shown in green), nuclear magnetic resonance (NMR; shown in red) and computational methods (shown in blue) are highlighted. MD, molecular dynamics; NaCl, sodium chloride; PDB, Protein Data Bank.

First structures in Structural Biology



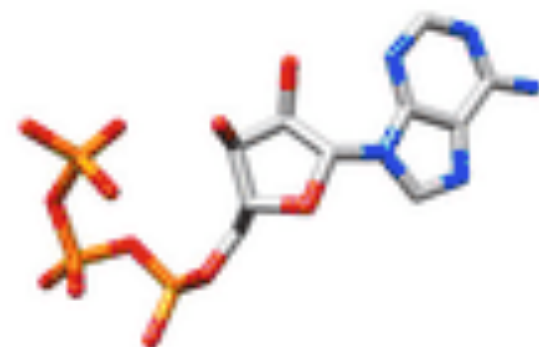
1962 of Max Perutz with his balsa-wood model of haemoglobin, and John Kendrew with his wire model of myoglobin. Models were derived from X-ray data. The resolution of the myoglobin data (1.4 Å). the haemoglobin data were derived at a lower resolution (6.0 Å).



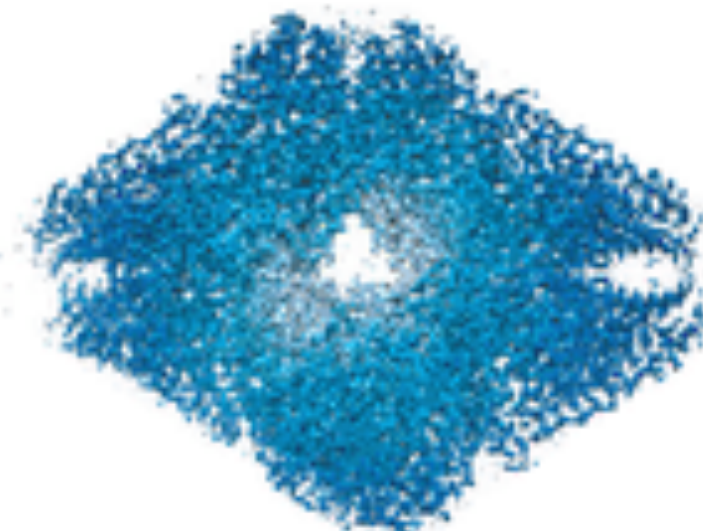
Nature Reviews | Molecular Cell Biology

Key Techniques in Structural Biology

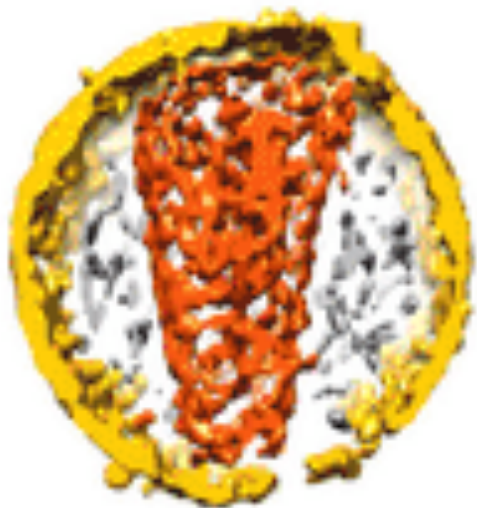
small molecules



proteins and protein complexes



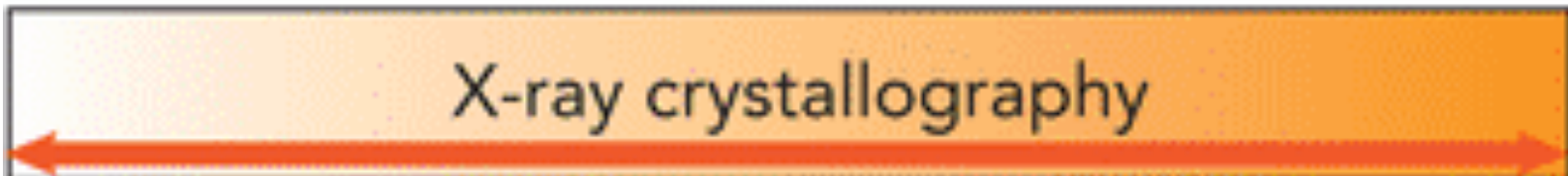
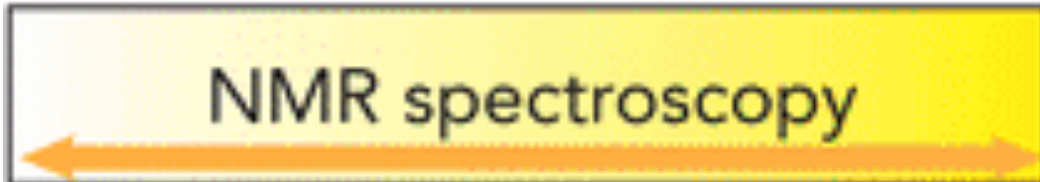
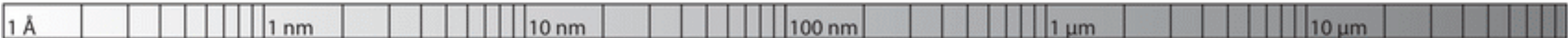
viruses and vesicles



Procaryotic cells and organelles

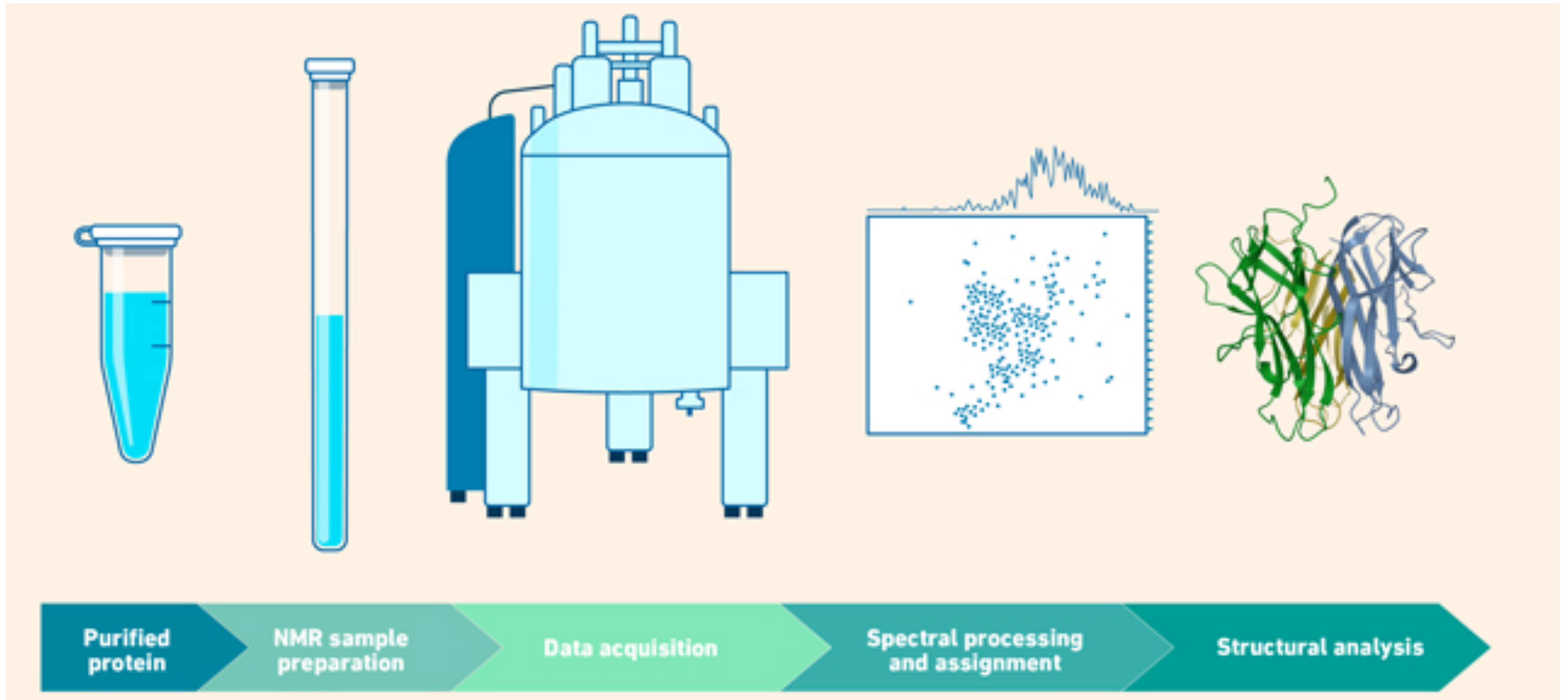


Eukaryotic cells



Size range of object investigated
Resolution attainable

Nuclear Magnetic Resonance



X-Ray Crystallography

Crystal



X-rays

Diffraction pattern



Processing

Electron density map



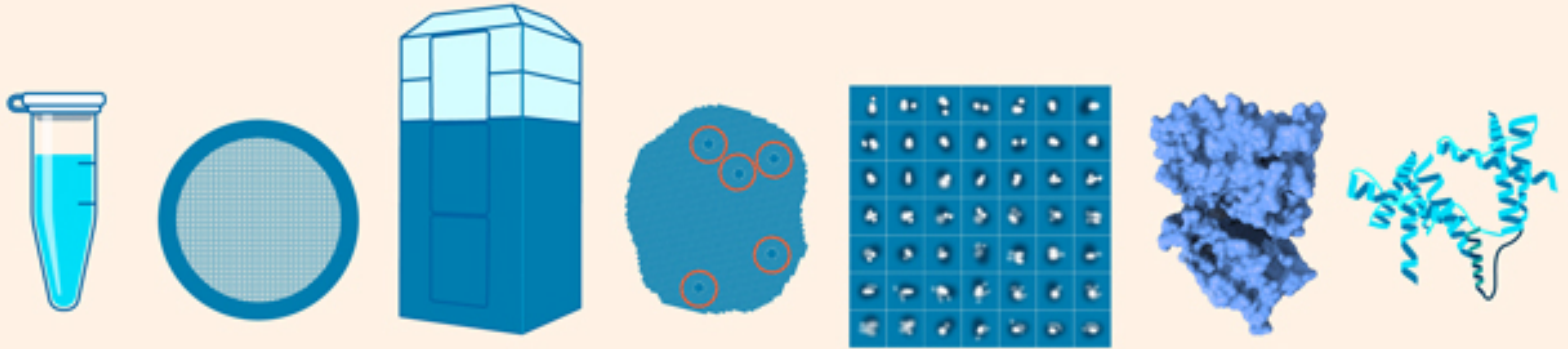
Fitting

Atomic model



Refinement

Cryo-electron microscopy



Purified protein

Freezing / Negative staining

EM data collection

Particle picking

Particle alignment and classification

3D model reconstruction

Model refinement

Protein Data Bank: The protein repository

Protein Data Bank: <https://www.rcsb.org/>

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RCSB PDB PROTEIN DATA BANK 215,908 Structures from the PDB 1,068,577 Computed Structure Models (CSM)

3D Structures Enter search term(s), Entry ID(s), or sequence Include CSM Advanced Search | Browse Annotations Help

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RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:

- Experimentally-determined 3D structures from the Protein Data Bank (PDB) archive
- Computed Structure Models (CSM) from AlphaFold DB and ModelArchive

These data can be explored in context of external annotations providing a structural view of biology.

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PDB-101 Training Resources

February Molecule of the Month

694 Structures 20 Unreleased Structures 274 Citations 140 Ligands 32 News & PDB-101 Articles

Search Parameter: Text Search for: hemoglobin

Refinements

ORGANISM

- Homo sapiens (254)
- Scapharca inaequivalvis (66)
- Amphitrite ornata (26)
- Equus caballus (18)
- Lupinus luteus (17)
- Cerebratulus lacteus (17)
- Physeter catodon (16)
- Other (280)

UNIPROT MOLECULE NAME

- Hemoglobin subunit alpha (310)
- Hemoglobin subunit beta (309)
- Globin-1 (64)
- Dehaloperoxidase A (24)
- Leghemoglobin-2 (17)
- Neural hemoglobin (17)
- Myoglobin (17)
- Refine Query

TAXONOMY

- Eukaryota (626)
- Bacteria (79)
- Other (1)

EXPERIMENTAL METHOD

- X-ray (676)

Currently showing 1 - 25 of 694 Page: 1 of 28

View: Detailed Reports: Select a Report Sort: Release Date: Newest to Oldest

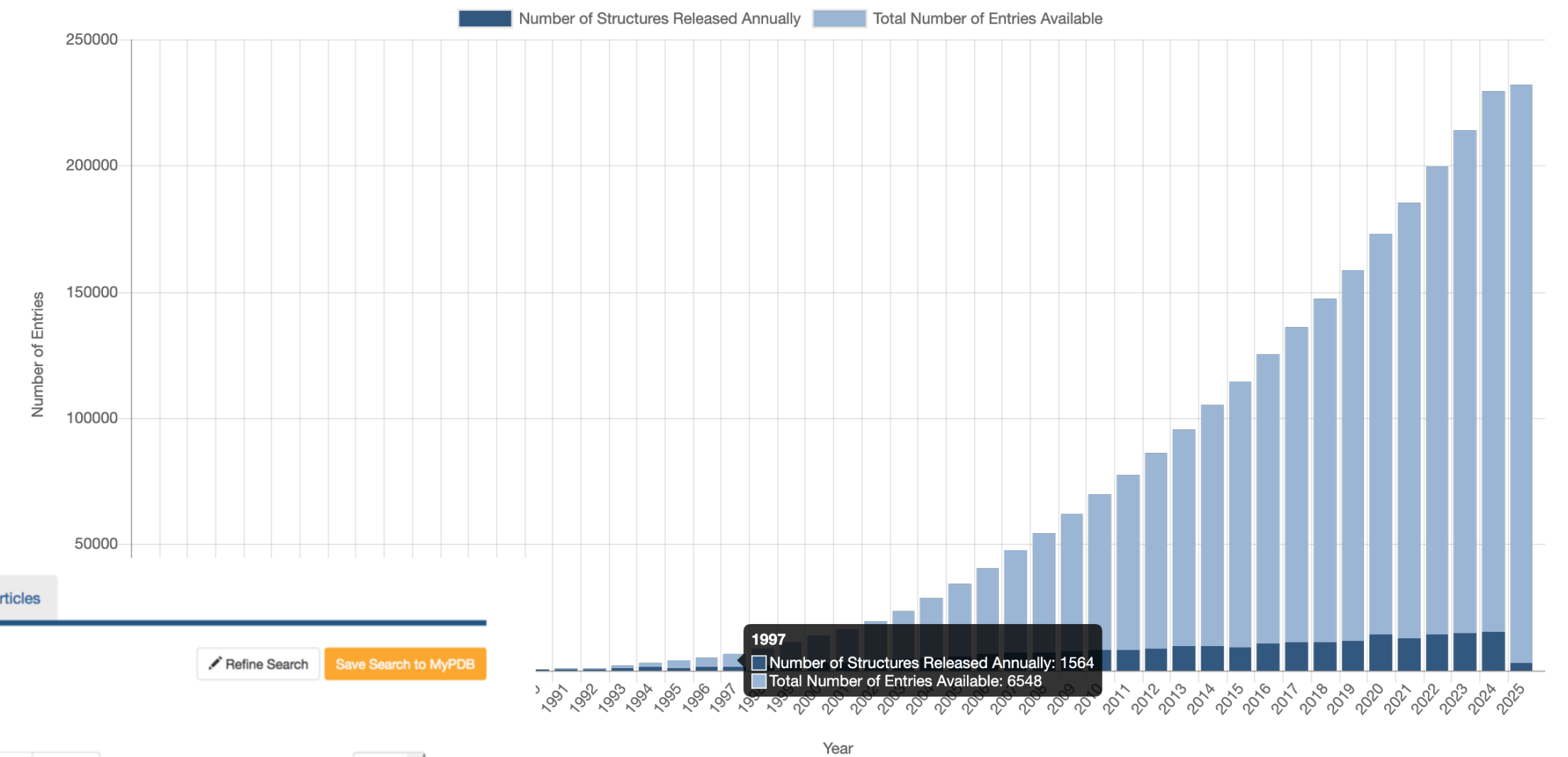
Structure of predicted ancestral pika hemoglobin

Inoguchi, N., Natarajan, c., Storz, J.F., Moriyama, H.

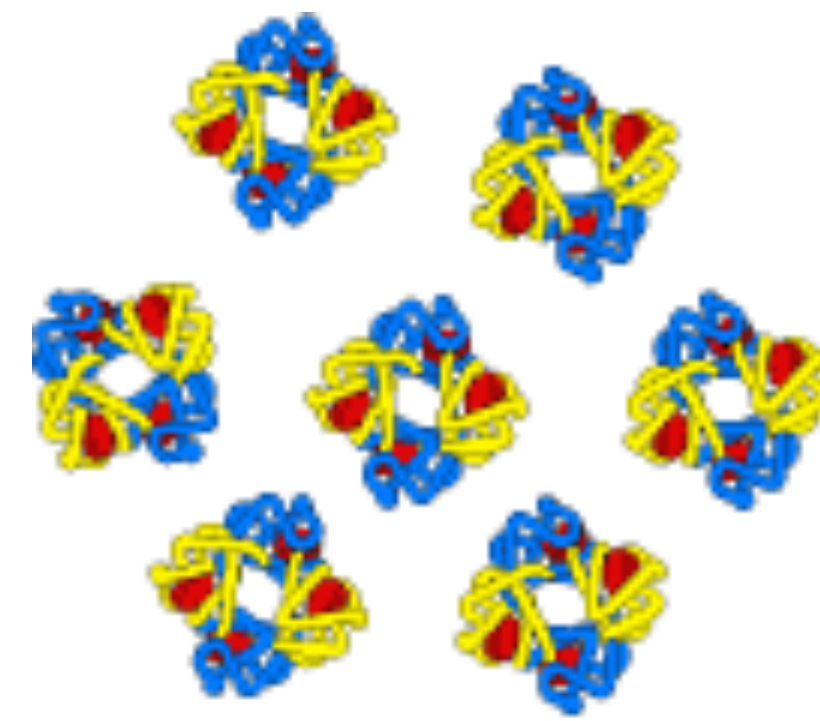
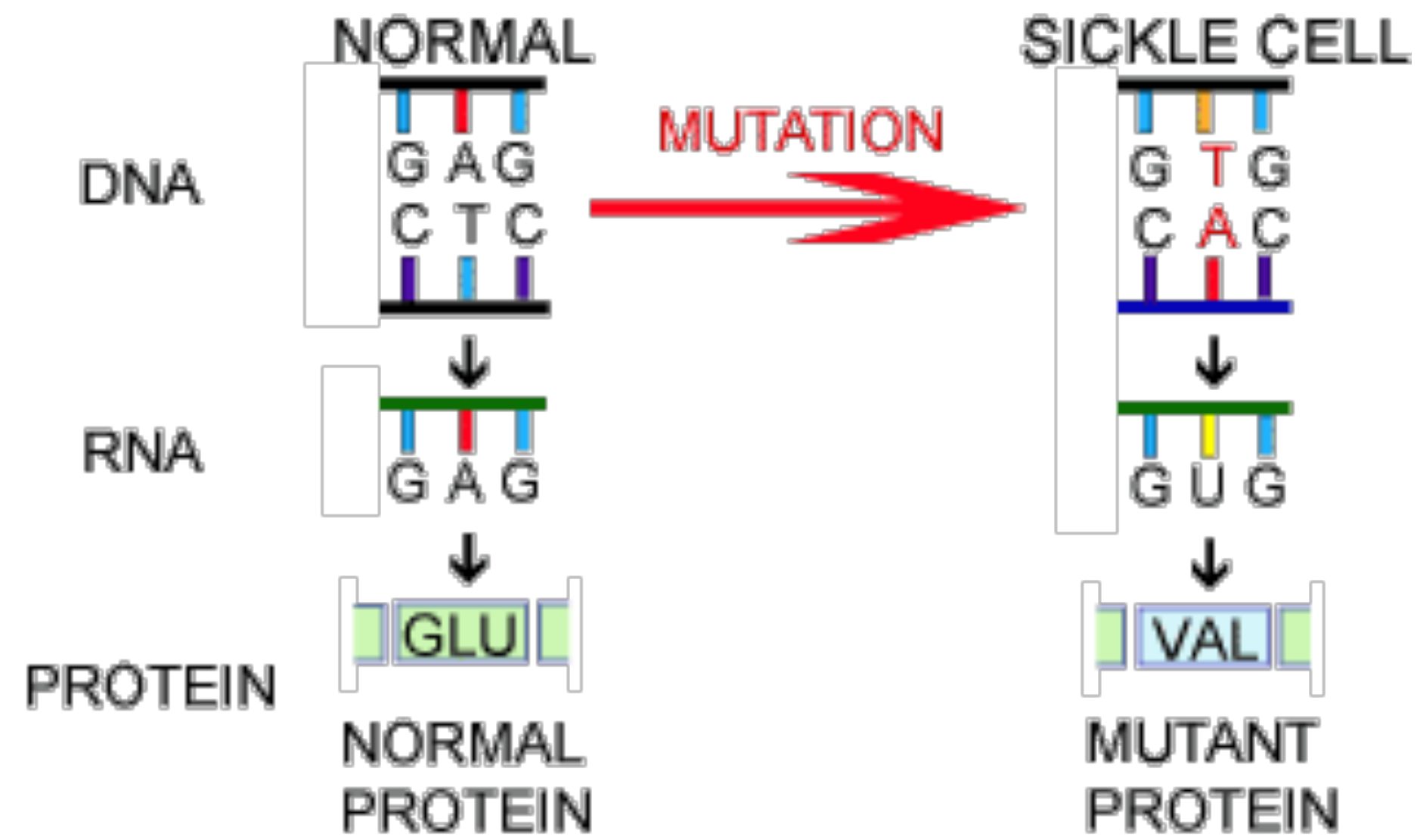
PubMed ID is not available.

Released: 11/30/2016 Method: X-ray Diffraction Resolution: 1.45 Å Residue Count: 287

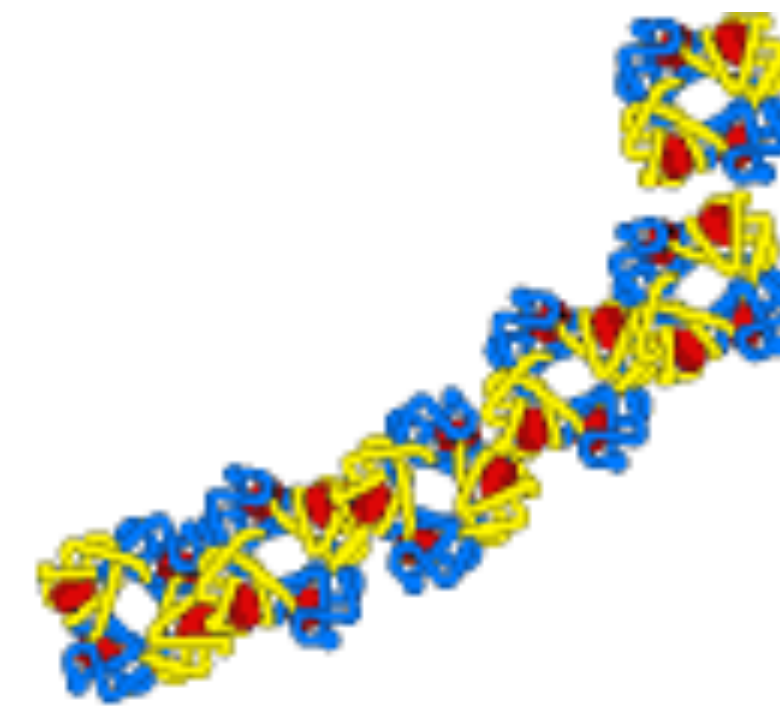
Macromolecule: HBA protein (protein) HBB protein (protein) Unique Ligands: HEM



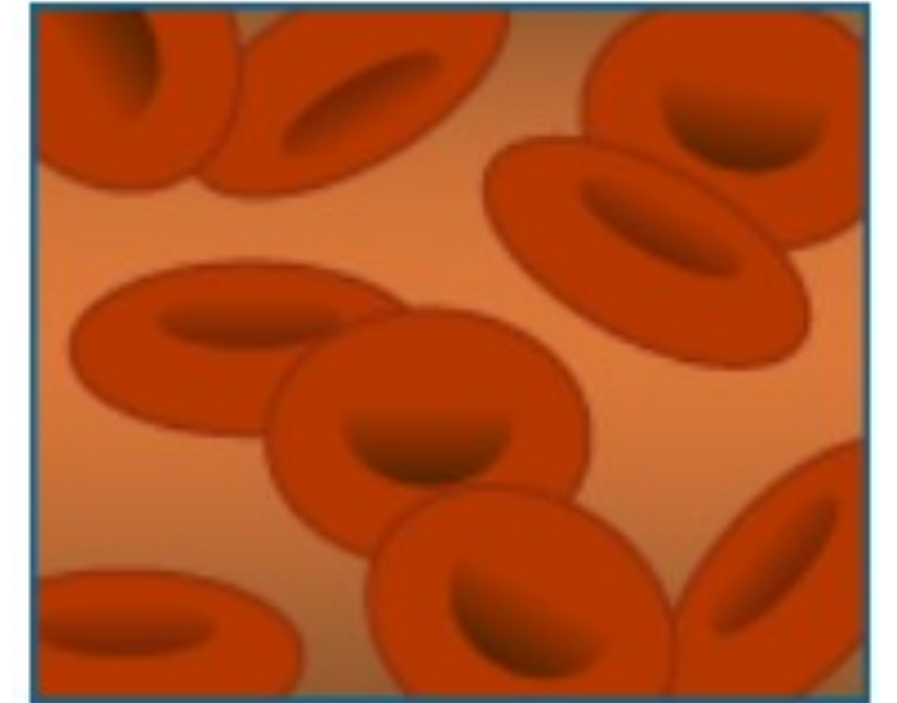
The impact of mutation on structure-function of protein



NORMAL HEMOGLOBIN

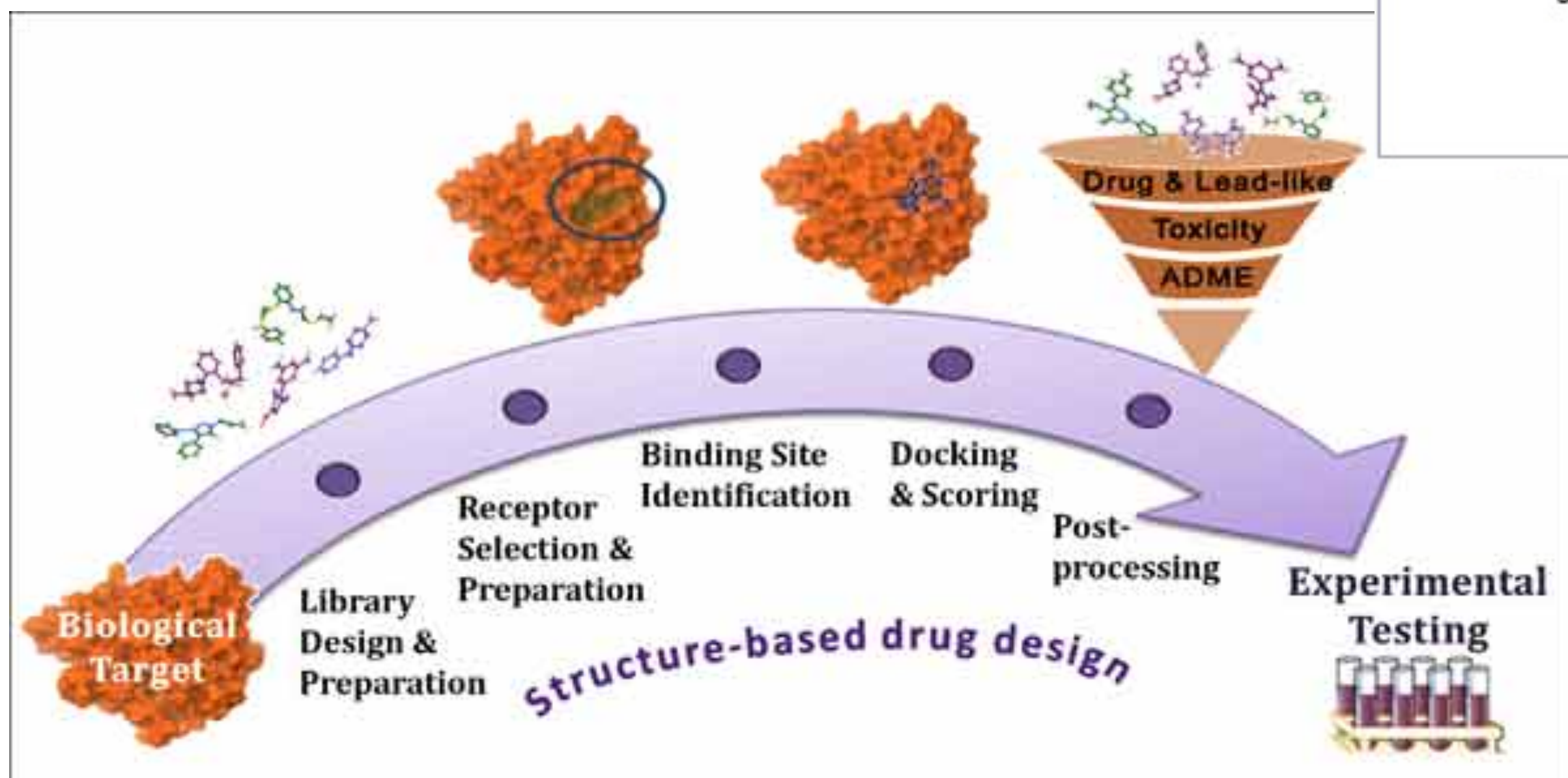
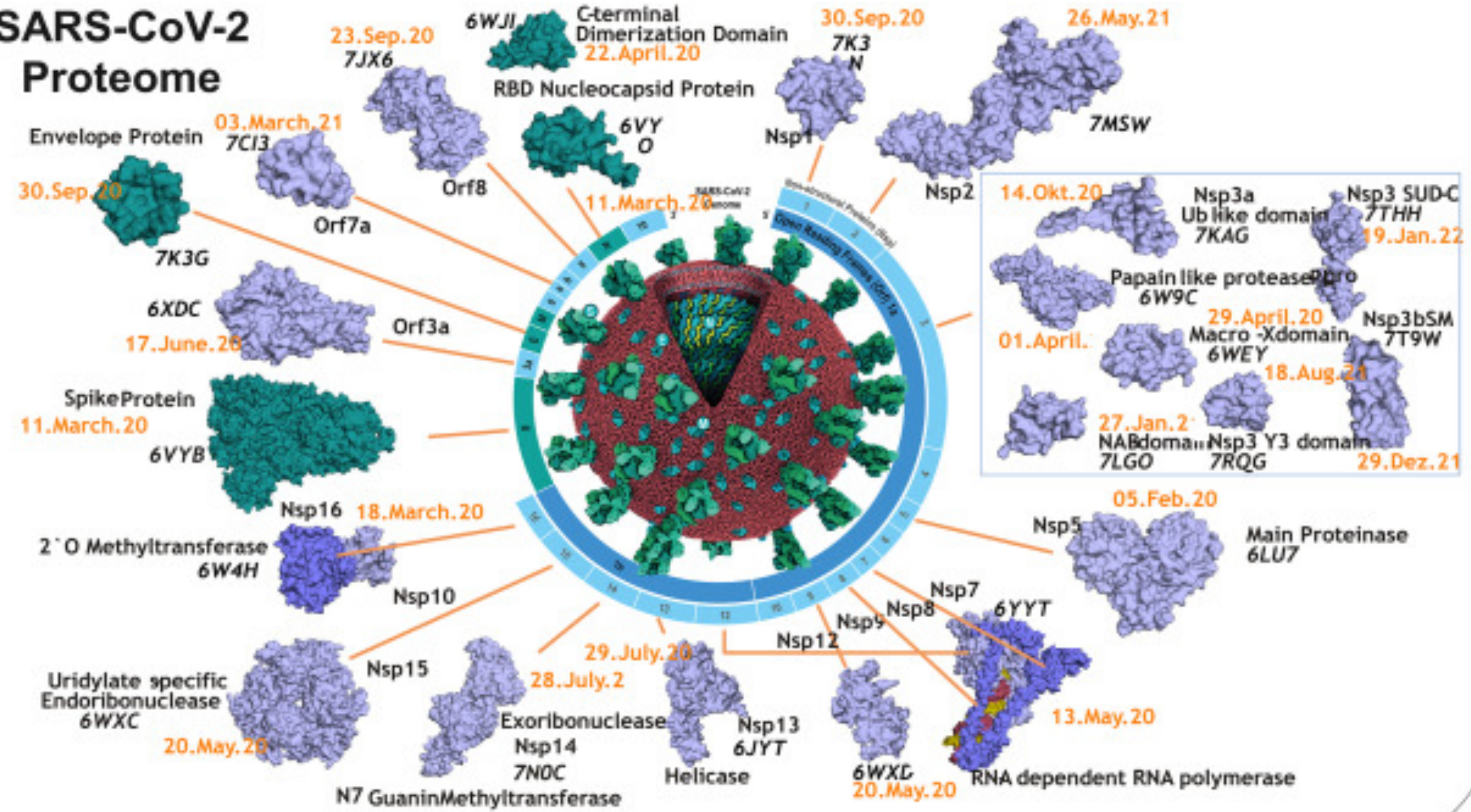


CLUMPED HEMOGLOBIN

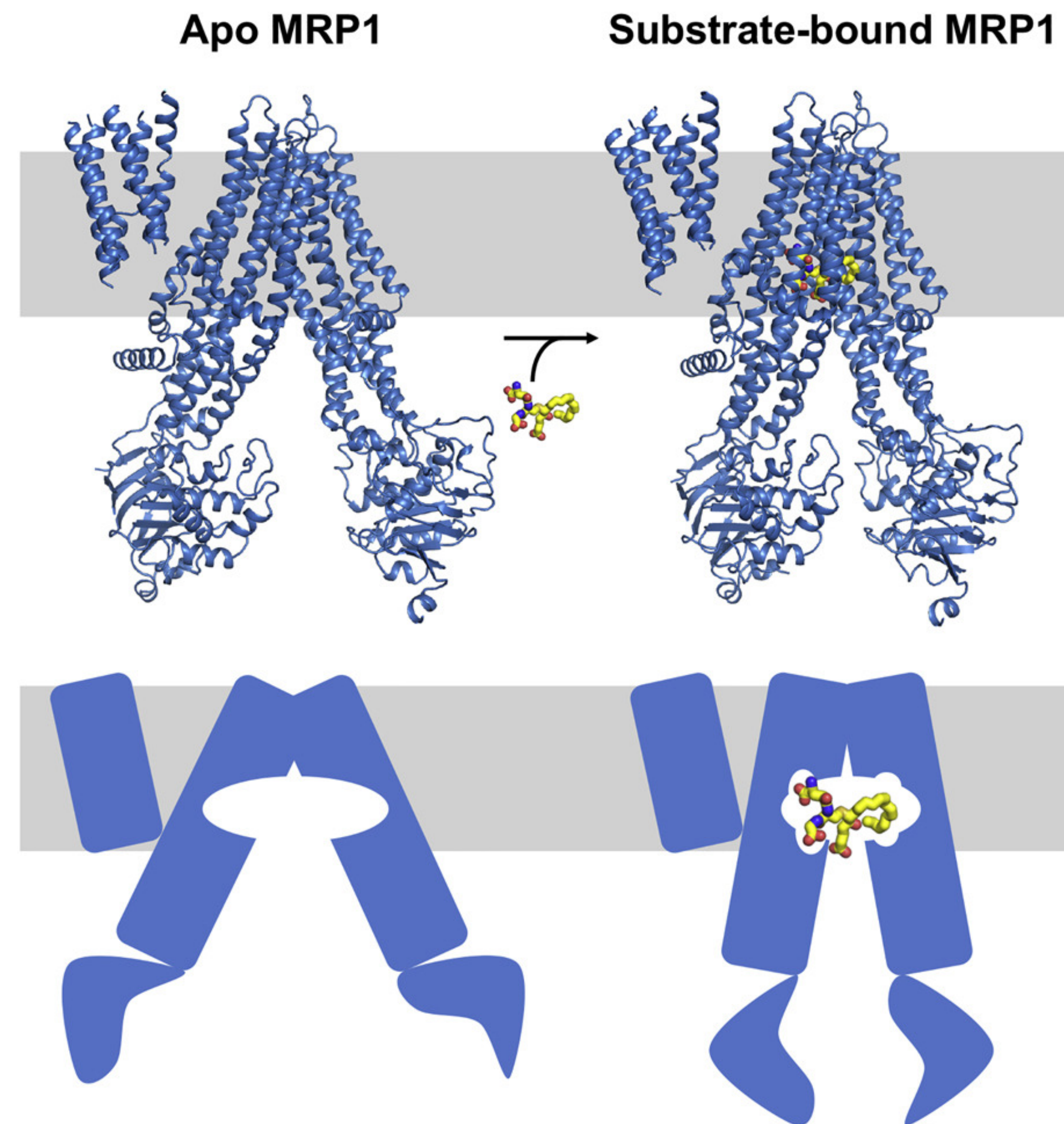


Structure-based drug designing

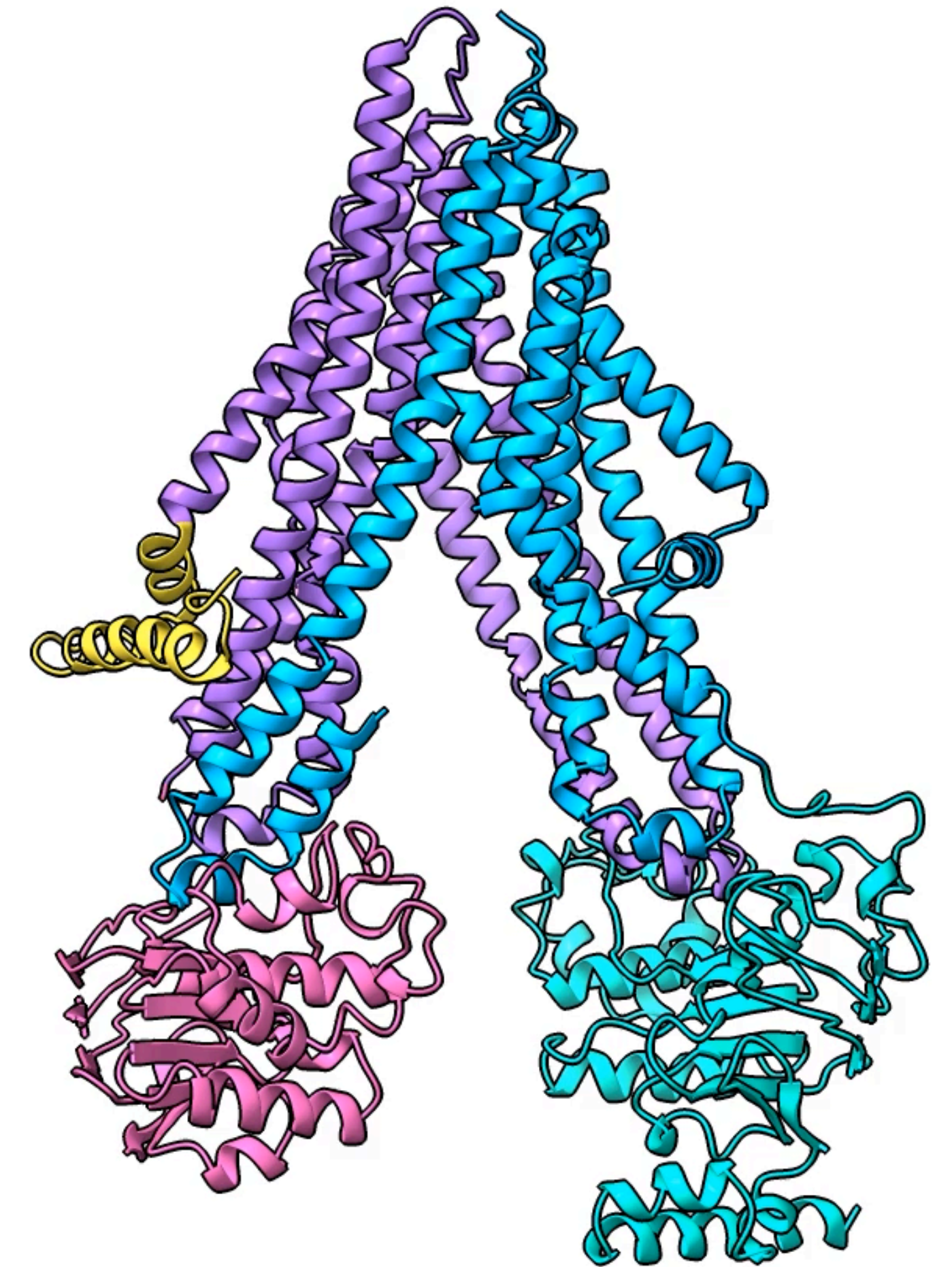
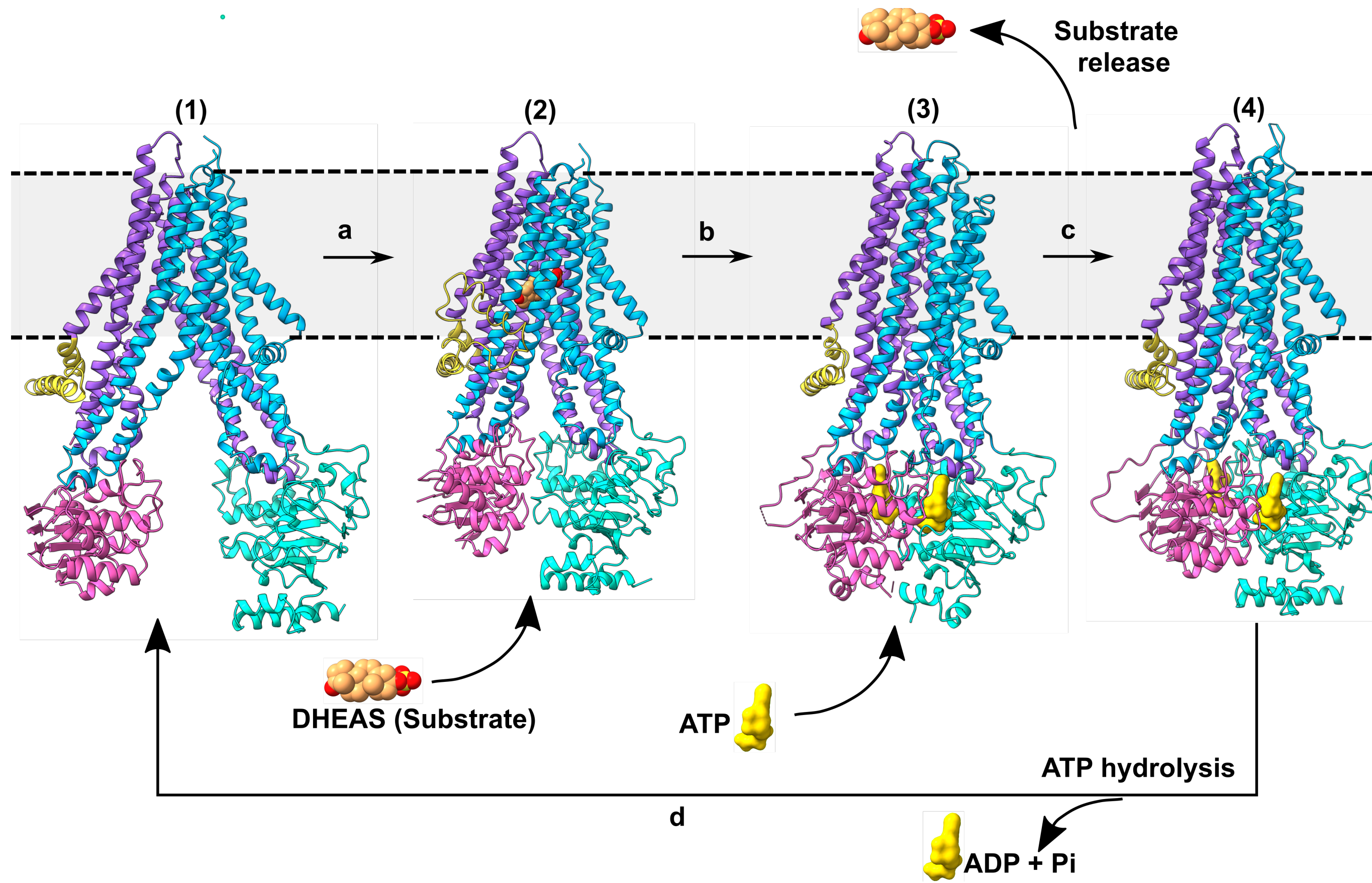
SARS-CoV-2 Proteome



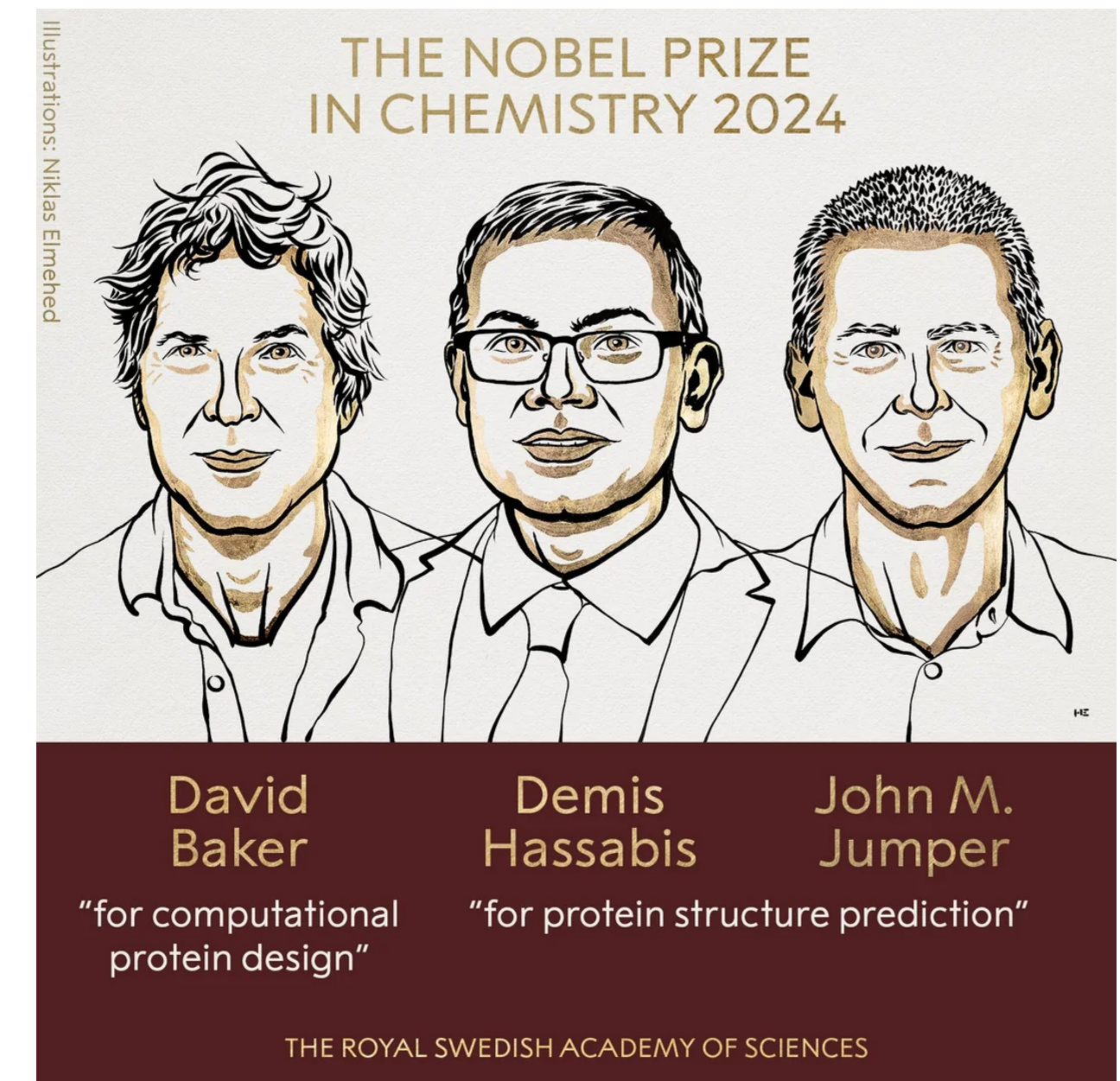
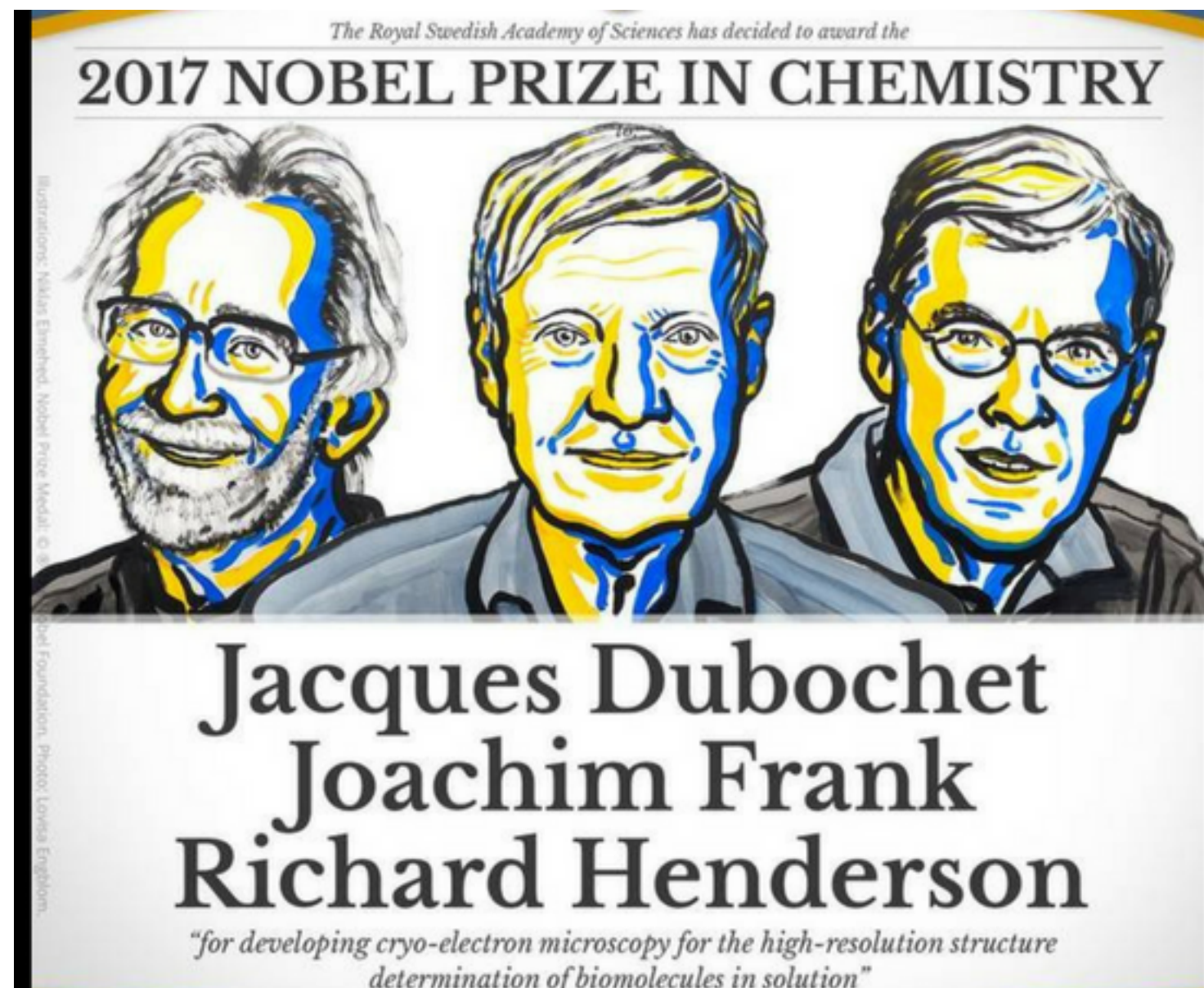
Conformational changes on ligand binding



Structure-functional relationships - catalytic cycle of protein



Recent Nobel prizes in Structural Biology



Questions