INTRODUCTION TO PROTEINS

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DIPARTIMENTO DI FISICA

SAPIENZA
UNIVERSITÀ DI ROMA

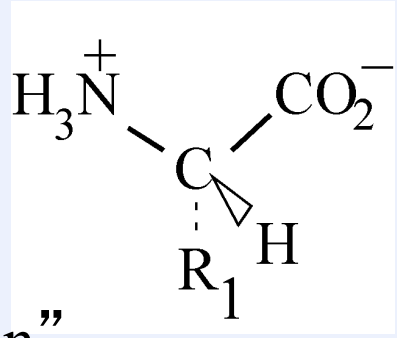
- SEQUENCE->STRUCTURE/UNSTRUCTURE->DYNAMICS-FUNCTIONS

JOURNALS
PROTEINS
PROTEIN SCIENCE
JOURNAL OF MOLECULAE BIOLOGY

Proteopedia https://proteopedia.org/wiki/index.php/Main_Page

Proteins

- From the Greek “proteios” meaning “of first importance”
- The basic building blocks of almost all living organisms
- Constitute the majority of the cell (see biology by numbers), and perform nearly all enzymatic activities
- Composed of 20 naturally occurring amino-acids



varying moiety called “side chain”

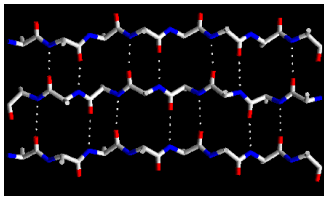
Hierarchy of Protein Structure

Primary 1°

AKSDQPWFAGLE

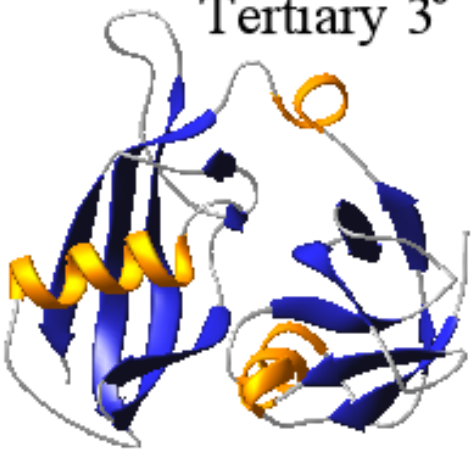
Linear chain made of 20 possible amino acids

Secondary 2°



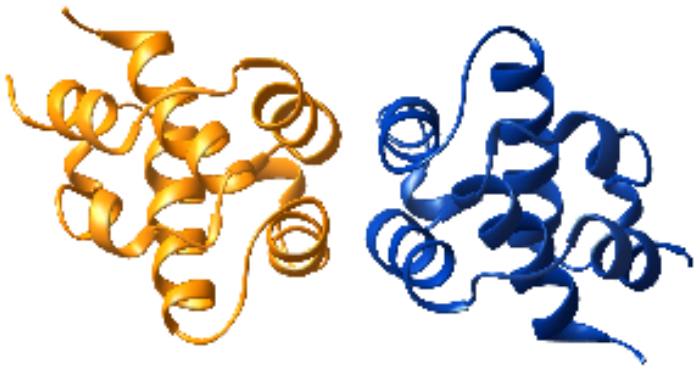
Alpha-helices, beta-sheets, tur

Tertiary 3°



Motifs, domains

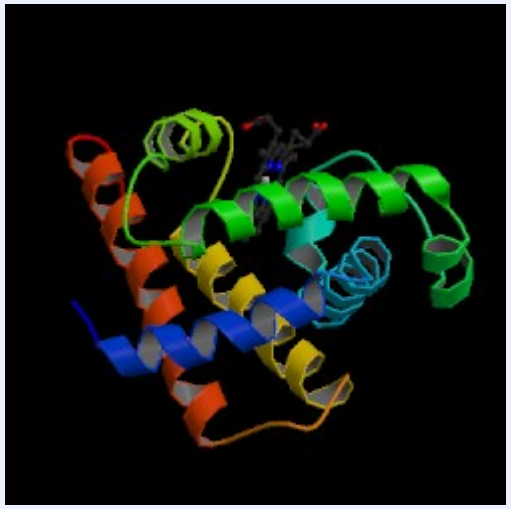
Quaternary 4°



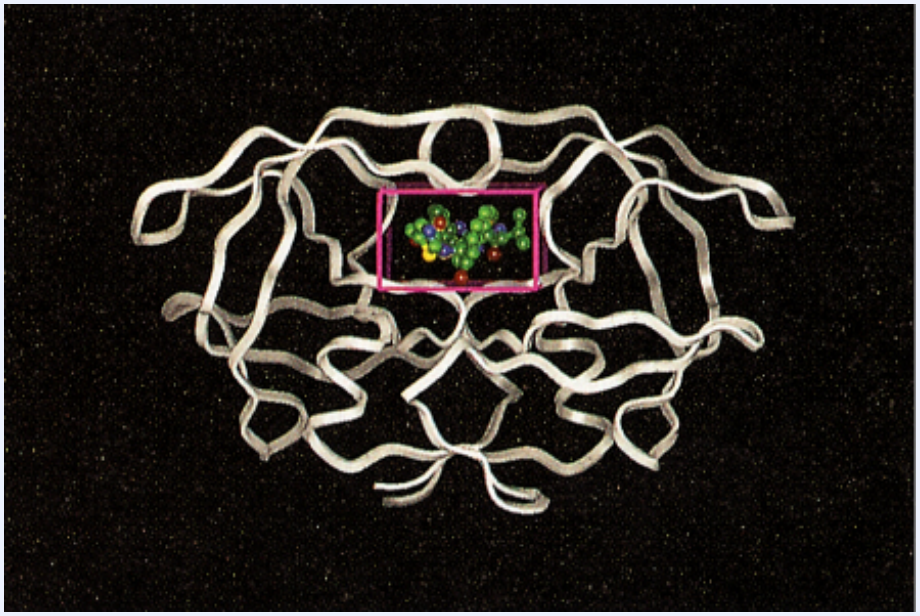
Oligomers, complexes

Structure/Unstructure

is quite basic in protein science

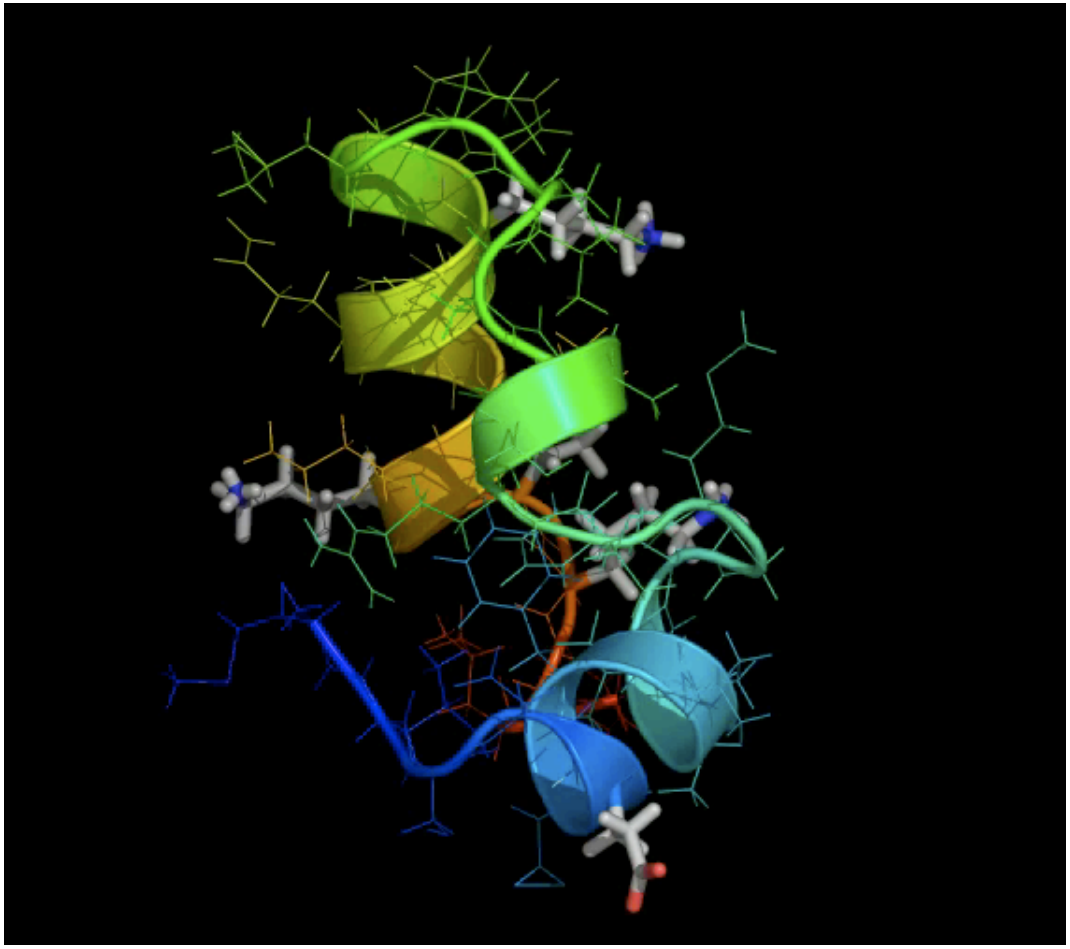


Myoglobin (1958) x-ray structure M.F. Perutz



Viral proteases are targets of the molecular design of inhibitor drugs such as Ritonavir, capable of blocking the active site of the enzyme and to contribute to the containment of HIV epidemics.

The Protein Data Bank (www.pdb.org)



Pioneers:
H. Frauenfelder, G. Careri,
G. Weber, (early seventies)
M. Karplus (1977)

Early review

Nature. 1990 Oct 18;347(6294):631-9.
Molecular dynamics simulations in biology.
Karplus M, Petsko GA..

Molecular dynamics--the science of simulating the motions of a system of particles--applied to biological macromolecules gives the fluctuations in the relative positions of the atoms in a protein or in DNA as a function of time. Knowledge of these motions provides insights into biological phenomena such as the role of flexibility in ligand binding and the rapid solvation of the electron transfer state in photosynthesis. Molecular dynamics is also being used to determine protein structures from NMR, to refine protein X-ray crystal structures faster from poorer starting models, and to calculate the free energy changes resulting from mutations in proteins.

Sequence->Structure->Function
Sequence->Function-> Structure
AND/OR DYNAMICS

Domain Boundaries, Reliability of Present Methods and Promising Avenues, Suggested Reading

Problem 3 Function Prediction
Introduction to the Problem, The Definition of Biological Function, The Function Vocabulary, Protein Names, Text Mining, Transferring Functional Annotations by Similarity, Transcriptomics, Proteomics, Promising Avenues, Suggested Reading

Problem 4 Protein Structure Prediction
Introduction to the Problem, Energetic Calculations of Protein Structures (Energy Calculation,

Water forms a hydration shell around proteins.

The properties of this bound water are still the subject of many experimental and theoretical investigations.