

# Protein Folding

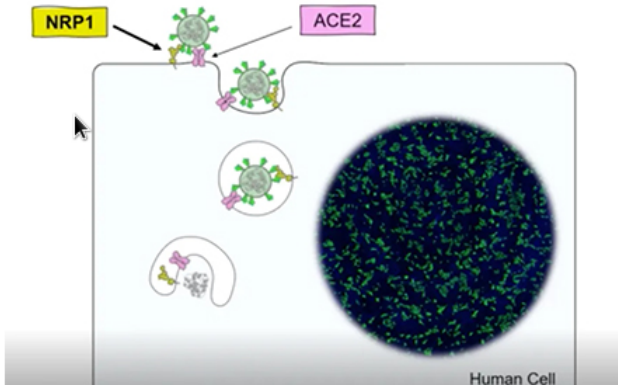
## Proteins, Aminos, Folding, and Trajectories

Luis Garreta

Electiva de Bioinformática  
MAESTRÍA EN INFORMÁTICA BIOMÉDICA  
Universidad del Bosque  
Bogotá-Colombia

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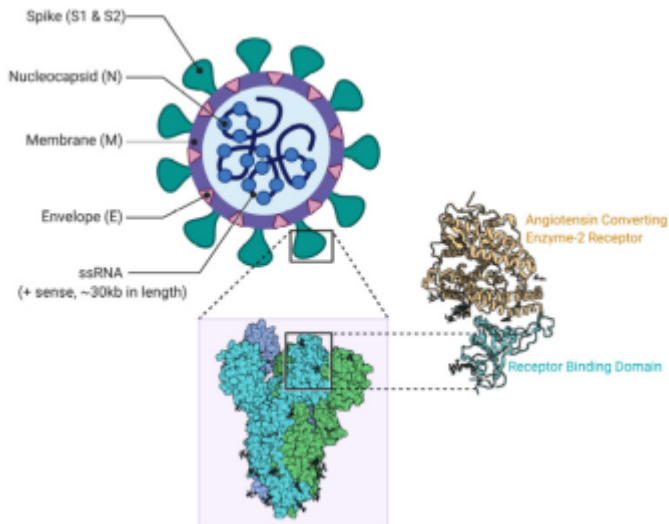
# SARS-CoV-2 enlace a la célula



# Simulación SARS-CoV-2 en acción

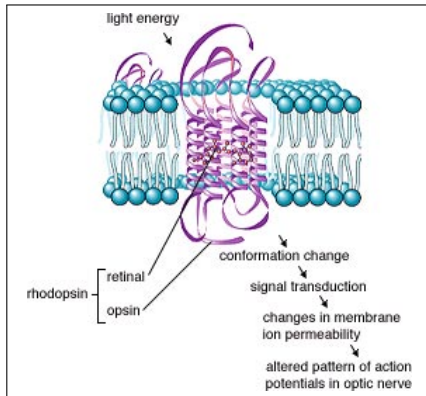
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# Estructura del SARS-Cov-2



# Importance of Proteins

- They are fundamental for life.
- Most important biomolecules
- Key roles in all living systems.
- They are part of
  - vision,
  - immune system,
  - muscles,
  - tissues,
  - ...
- They are in all of our body.

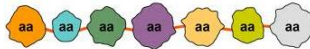


# What are Proteins ?

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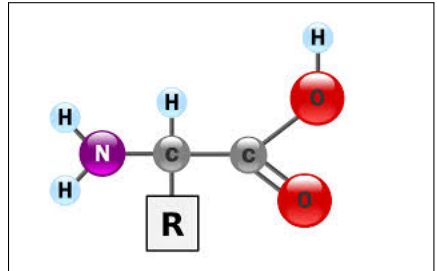
# What are Proteins ?

A sequential chain of amino acids



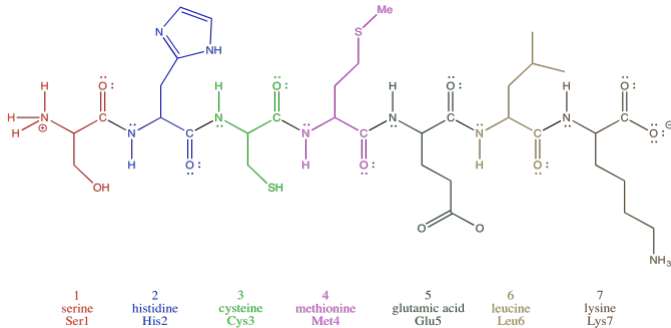
# Amino acids

- Aminoacid is composed by atoms:
  - Carbon,
  - Oxygen,
  - Hydrogen, and
  - Nitrogen



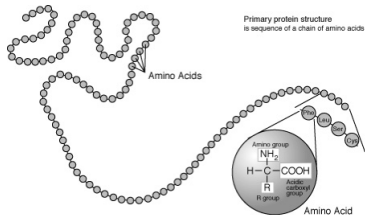


# Sequence of aminoacids



# Sequence of aminoacids

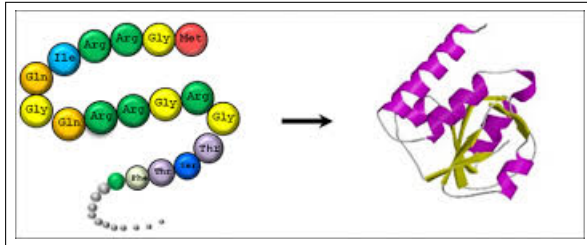
- Primary protein structure is a **sequence of aminoacids**



- A necklace of beads
- Each bead is an amino acid
- Amino acids have an structure

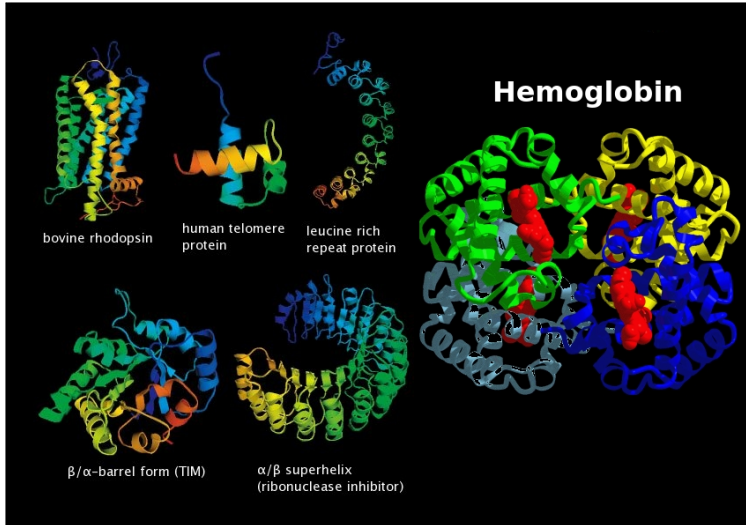
# Proteins fold in tridimensional shapes

- Proteins can take many 3D structures (shapes)



- The shape is associated with the function

# Examples of Proteins



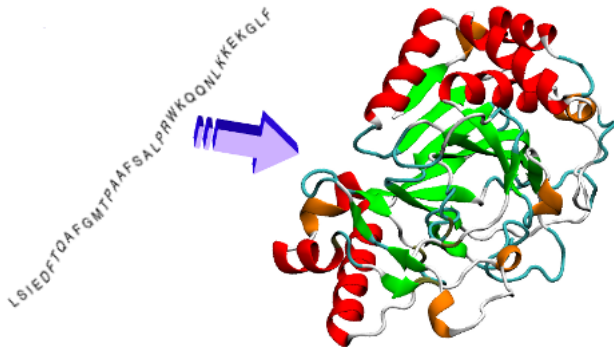
[https://figshare.com/articles/Hemoglobin\\_is\\_a\\_Flexible\\_Protein\\_NMR\\_Structure\\_2M6Z\\_7903674](https://figshare.com/articles/Hemoglobin_is_a_Flexible_Protein_NMR_Structure_2M6Z_7903674)



# How do proteins fold?

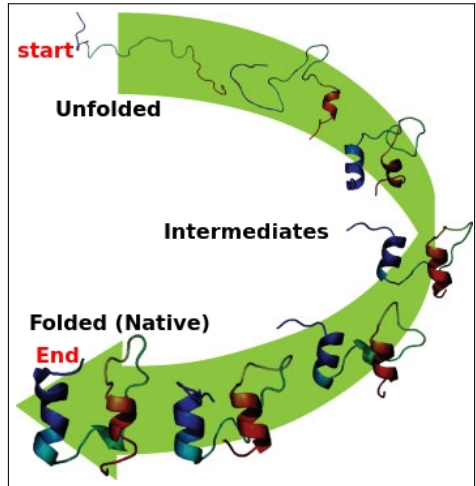
# Protein Folding Problem

Proteins fold from a linear sequence of amino acids to a 3D structure



# Protein Folding Process

- Complex process in biology
- Hard to understand by scientist
- **Challenge** for biologists, biophysics, and computer scientists
- Very Important:
  - Medicine
  - Drugs discovery
  - Treatment of diseases
  - Among others...

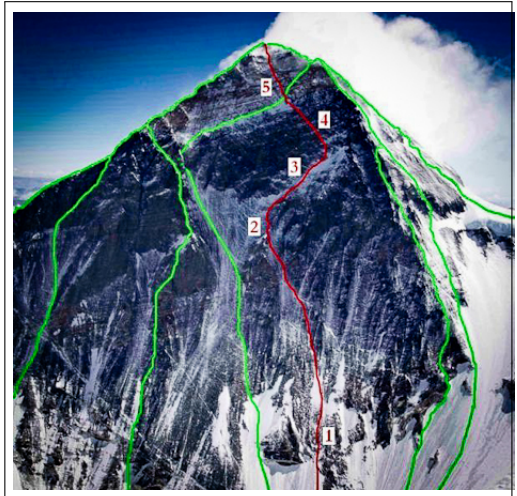


# Protein Folding as Mountain Climbing

Bottom: unfolded state

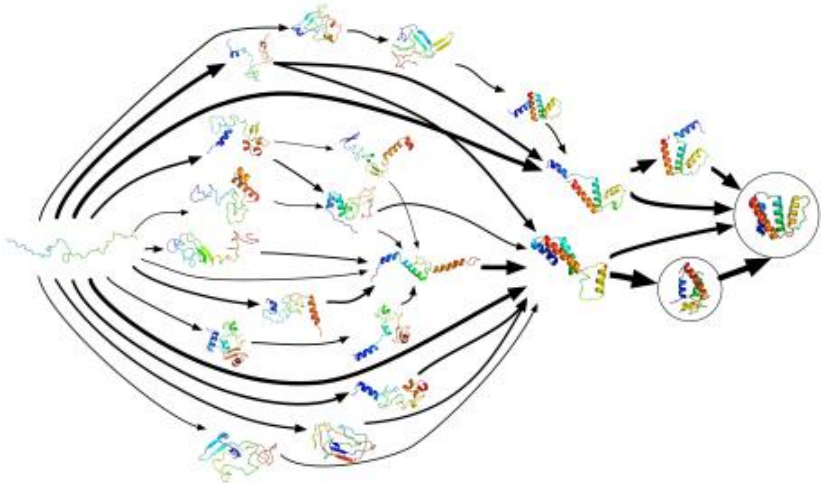
Points : intermediate states

Top : folded or native state

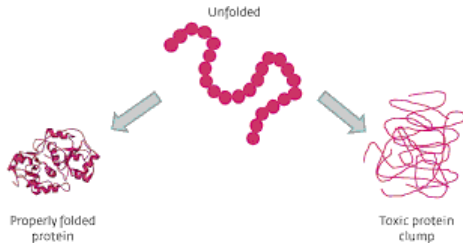




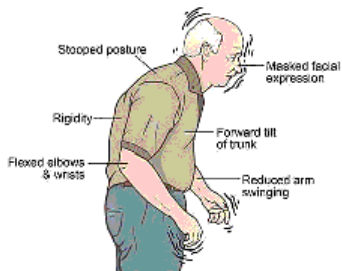
# Protein Folding Pathways



# Folding and Misfolding



Typical appearance of Parkinson's disease



# Protein Folding Simulation using Molecular Dynamics

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