

# Protein Folding Simulations

## Proteins, Aminos, Folding, and Trajectories

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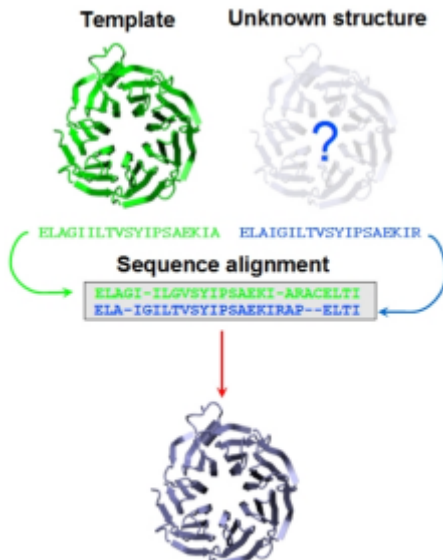
Electiva de Bioinformática  
MAESTRÍA EN INFORMÁTICA BIOMÉDICA  
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Bogotá-Colombia

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# Protein Structure Prediction Methods

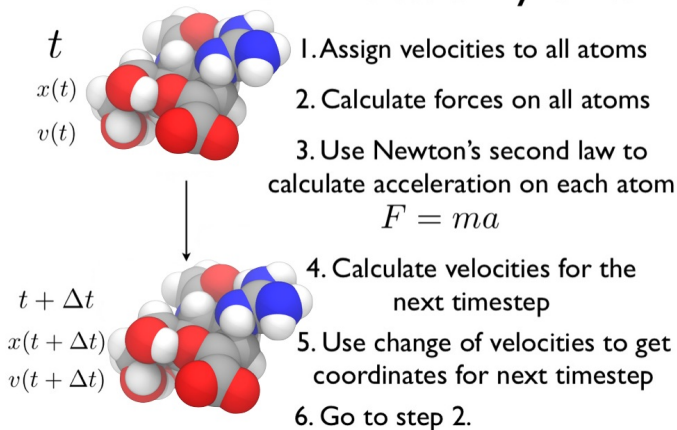
- Homology modeling
- Fold recognition
- Fragment Assembly
- Molecular dynamics

# Homology Modeling

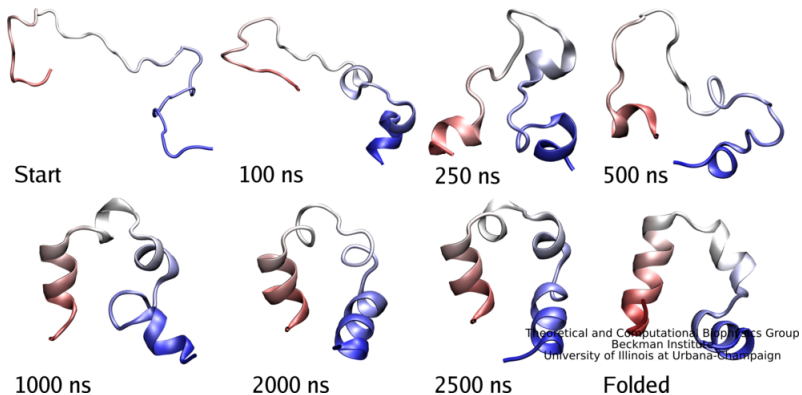


# Protein Folding Simulations

## Molecular Dynamics

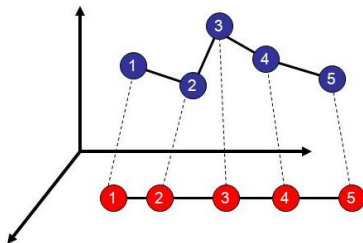


# Protein Folding Simulations

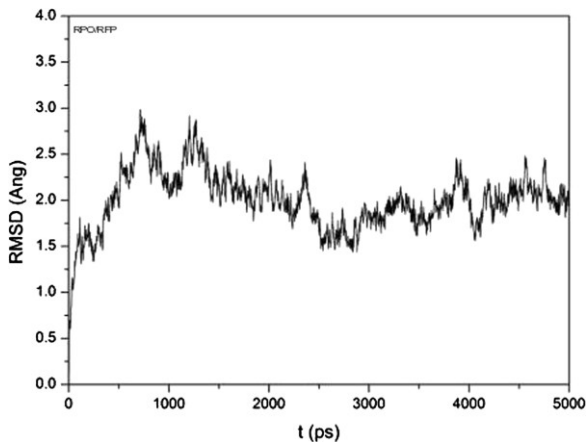


# Comparison between structures

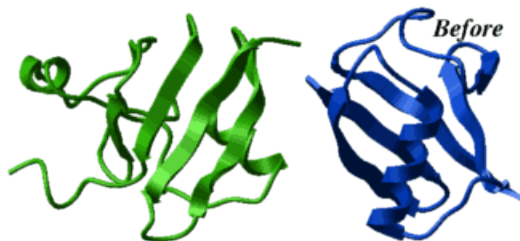
Using RMSD to find the optimal superposition



# Protein Folding Trajectories



# Protein Comparison

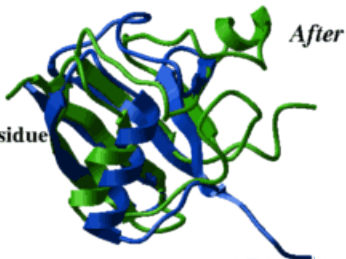


align a\_1.1 a\_2.1



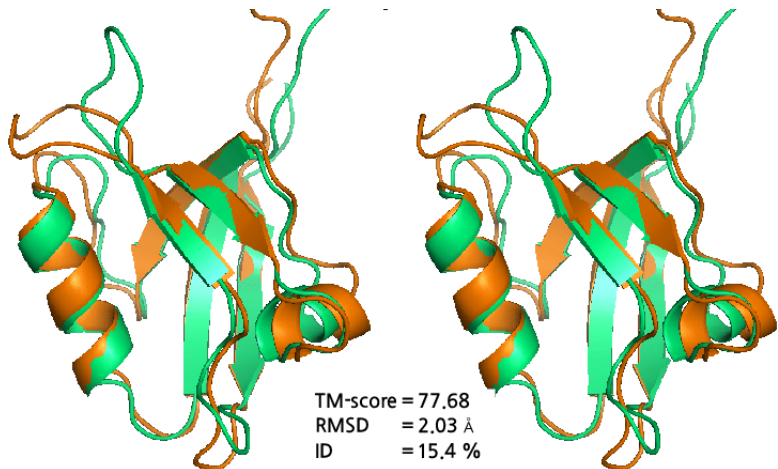
Result:

- 1) superposition
- 2) Two equiv. residue selections





## Metrics for Protein Comparison



RMLPRLCCLEKGPNGYGFLHGEKG---KLGOYIRLVEPGSPA-E-KAGLLAGDRLVEVNGENVEKETHQQVVSRIIRAALNAVRLLVDPETDEQL----  
GAIITYVELKRYGGPLGITISGT--EPPFDPIIISSLTKGGLAERTGAINIGDRILAINSSSLKGKPLSEAIHLLQAGETVTLKIKKQTDQA--PASS