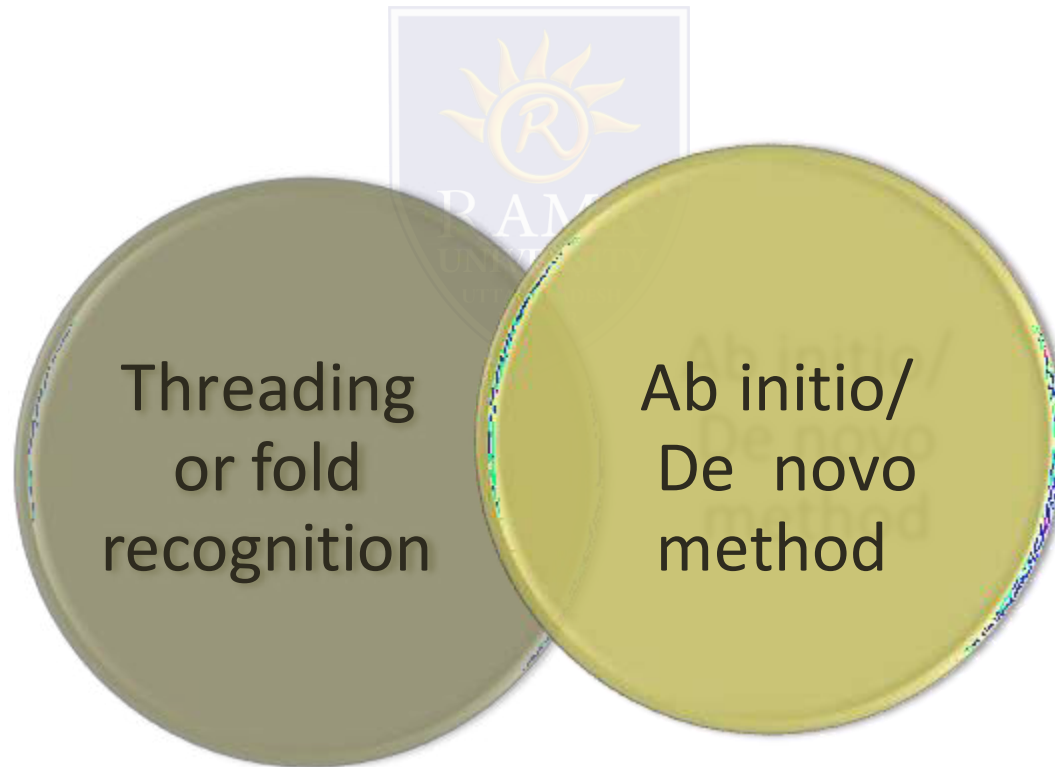




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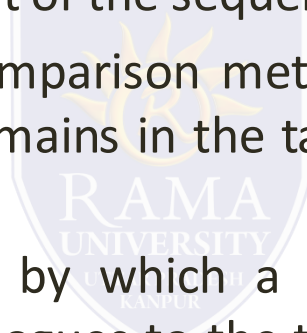
**Department of Biotechnology**

## Methods of protein structure and modeling

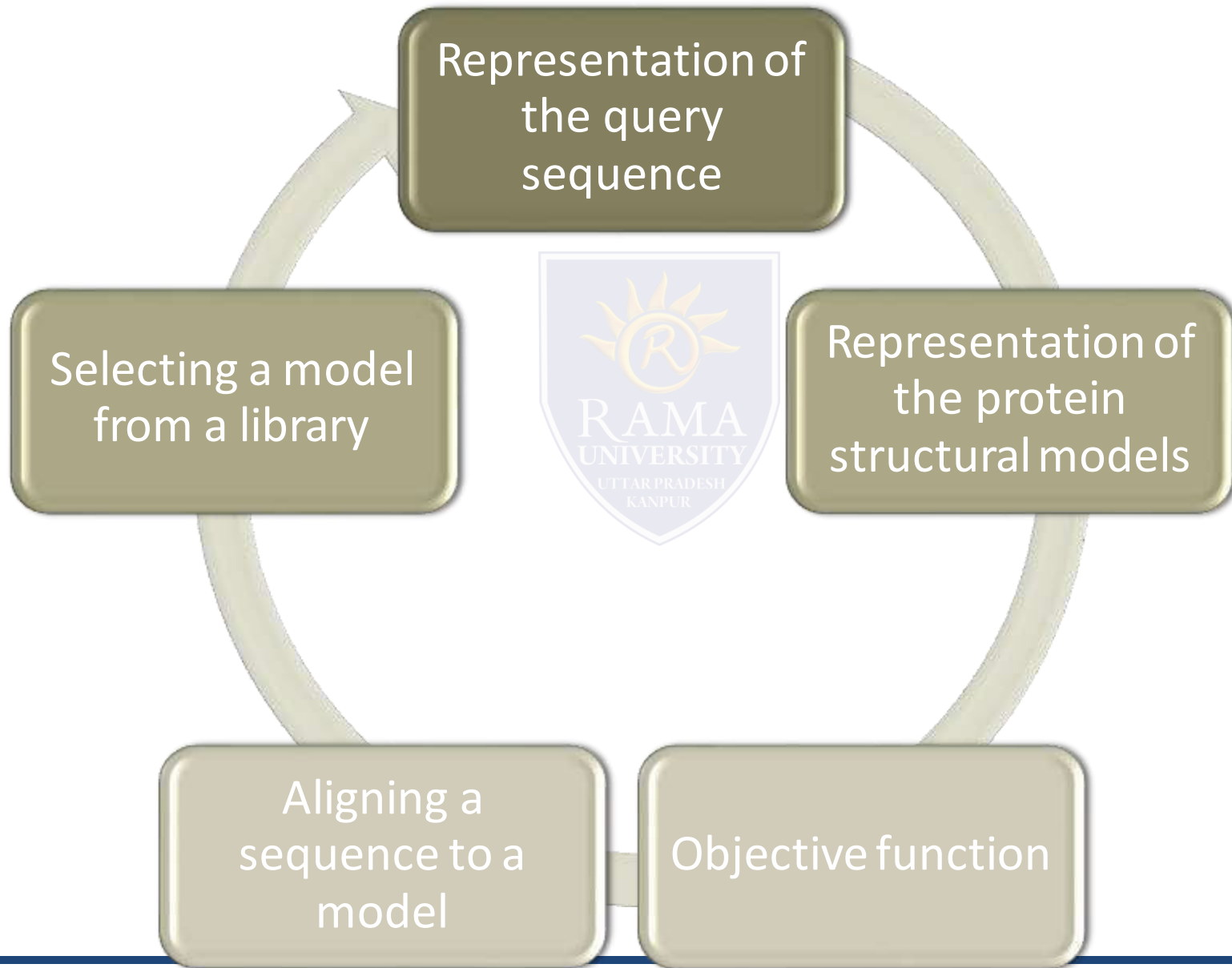


# Threading

- There might be a structural similarity in two proteins with almost less than ten percent of the sequence similarity
- When sequence based comparison methods are not much efficient to recognize the folds and domains in the target sequence then we proceed with the threading
- Threading is the method by which a library of unique structures is searched for structure analogues to the target sequence, and is based on the theory that there may be only a distinct number of folds

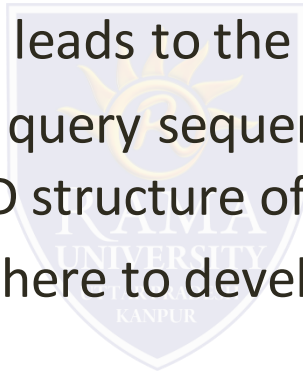


# Basic components of folding



# Representation of the query sequence

- Similar protein sequence leads to the similar protein structure
- Sequences similar to the query sequence are carrying information about the 3D structure of the query sequence
- The algorithms are also there to develop the different representation

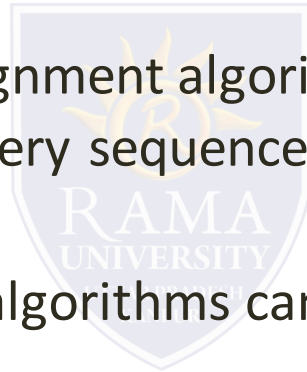


# Objective function

- The 3D data deposited in the databases like PDB is analyzed via the different statistical protocols
- These analyzed data are now referred to as knowledge based potentials or empirical potentials
- In the case of non-linear models the other name is contact potentials etc

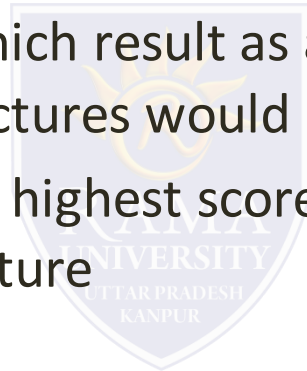
# Aligning a sequence to a model

- The goal of threading alignment algorithm is to find an optimal match for the query sequence to the best suited sample protein sequence
- The sequence structure algorithms can be done to find the best suited match



# Selecting a model from a library

- The different models which result as a base of alignments of the sequences and structures would lead to multiple results
- The best result with the highest score would be selected to model the protein structure





# Ab initio method

- Ab initio structure prediction leads to the protein structure determination by the protein sequence alone
- The free energy estimation of all the molecules present in the amino acid sequence of the protein is also done independently
- The two key components of the de novo methods are the procedure for the efficiently carrying the conformational search and the free energy estimation function used for evaluating the possible conformations.

# Ab-initio method

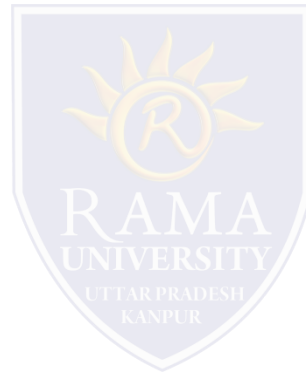
## Advantages

- Ab-initio approach can be applied to model any sequence

## Disadvantages

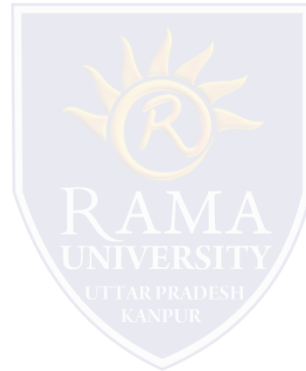
- Low resolution models
- Limited number of residues of less than 100 amino acids could be modeled only





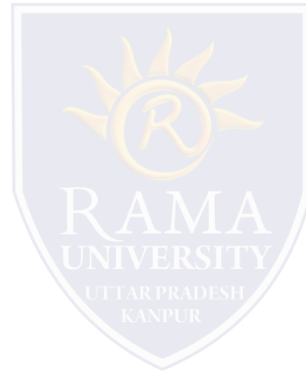
XYZ

abc



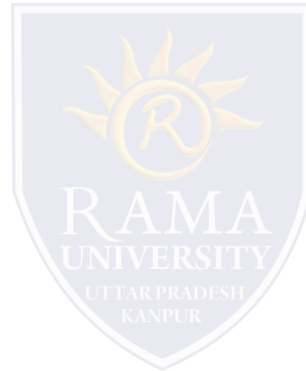
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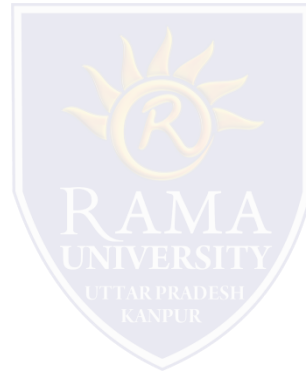
XYZ

abc



XYZ

abc



# MCQs

1. A
2. A
3. A
4. A
5. A
6. A
7. A
8. A
9. A
10. A

