RAMA
UNIVERSITY

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FACULTY OF ENGINEERING AND TECHNOLOGY

Department of Biotechnology

Secondary structure prediction

In Secondary Structure Prediction, We will get three dimensional structure of protein, from that three dimensional structure we will get the function of the specific protein.

Secondary Structure Prediction are devised by many tools.

Chou-Fasman method

GOR (Garnier, Osguthorpe and Robson) Method Nearest

SOPMA (self-Optimized Prediction method based on MSA)

METHODS OF SECONDARY STRUCTURE PREDICTION

- ✓**Chou- Fasman methods**
- ✓**GOR methods**
- ✓**Nearest neighbour methods**
- ✓**Hidden Markov models**
- ✓**Neural networks**
- ✓ **Multiple alignment based self optimization method**

ALPHA HELIX MAKERS:

Alanine

Glutamine

Leucine

Methionine

ALPHA HELIX BREAKERS:

Proline

Glysine

BETA SHEET MAKERS:

- **Isoleucine**
- **Valine**
- **Tyrosine**

BETA SHEET BREAKERS:

- **Proline**
- **Asparagine**
- **Glutamine**

PROPENSITY VALUE

- **Tendency of the aminoacids to behave more in alpha helix and beta sheet.**
- **Propensity value for Alpha Helix =**

Frequency of amino acids in Alpha helix

Frequency of residues to be in Alpha helix

If Alpha helix is made up of 20 amino acids and amino acids present for 5 times ,

Frequency of amino acids = 5/20= 0.25

If the total 100 residues in the protein, but only 20 makes
the Alpha helix,
Frequency of residues to be in the helix =20/100=0.2

This is applicable for beta sheets also.

Rule for Alpha helix formation:

- Firstly, we have to scan 6 amino acid residues at random.
- Then look for maker and breakers
  - If there is more than 1/3 of breaker, there is no helix formation.
  - If there is less than 1/2 of makers, there is no helix formation.
- Naturally it adding the stretch of sequence till the propensity value of helix is greater than OR equal to 100.
- Four such amino acid have propensity value of helix is greater than 100, it terminates the elongation.
- There are 9 amino acid sequence with more maker and less breaker make Alpha helix.
- Negative charged amino acid at N terminal and
- Positive charged amino acid at C terminal form the ALPHA HELIX.

- ✓ If propensity value for Alpha helix is greater than OR equal to 1.03, form the ALPHAHELIX.
- ✓ Alpha helix makers should be greater than Alpha helix breakers.
- ✓ The propensity value of Alphahelix should be greater than the propensity value of Beta sheet.

Rules for Beta Sheet formation:

- ✓ Firstly, we have to scan 5 amino acid residues at random.
- ✓ If propensity value for Beta sheet is greater than OR equal to 1.05, form the BETA SHEET.
- ✓ Other rules are as same as Alpha helix formation.

GOR METHOD

- ✓ GOR method assumes that amino acids up to 8 residues on each side influence the secondary structure of the central residue.
- ✓ This program is now fourth version.
- ✓ The accuracy of GOR when checked against a set of 267 proteins of known structure is 64%.
- ✓ This implies that 64% of the amino acids were correctly predicted as being helix, sheet or coil.
- ✓ The algorithm uses a sliding window of 17 amino acids.

NPS@ _GOR4 SECONDARY STRUCTURE PREDICTION RESULTS.pdf

XYZ

abc

XYZ

abc

XYZ

abc

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