International Journal of Multidisciplinary Allied Research Review and Practices

IJMARRP ISSN No: 2455-1570 (Volume 3, Issue 7, July 2016)

Study of congenital heart disease, Parkinson's and haemolytic aneamia with the help of protein structure prediction method HMM using Bioinformatics

Talib Yusuf*, Talib S.H.**, Amruta Mane***

*Department of Biotechnology, MGM University of Health Sciences, Aurangabad.

**Department of Medicine, MGM Hospital and Medical College, Aurangabad.

***Department of Biotechnology, Institute of Science, Mumbai

Abstract

Protein structure prediction is one of the method by which we can predict the helix, sheets and threads available on protein complex molecule. HMM (homology Molecular Modeling) is one the method classified in 3D structure prediction provides you the important aspects of protein molecule and stand of that fragment on evolutionary tree. These protein structure prediction methods also help us to deal with information provider for disease level we can predict their binding sites in molecule. In these paper we tried to study some diseases using there protein molecule for study there work and cycle in disease causing our aim is to find out the template for the protein molecule for which we are studying of disease like Heart disease, Parkinson's and Haemolytic anaemia. The quality of the HMM depend on the quality of the sequence alignment and template structure.

I. Introduction

Proteins are made up of long chains of amino acid residues which have the ability to perform various functions like DNA replications, responding to stimuli, and transporting molecules from one place to another and other various functions. Proteins are dictated and messaged by nucleotide sequences of their genes that makes differ from one protein to another. To study these different aspects researcher try to study the different dimensions of protein implementing the different methods of structure predictions. In these paper we tried to study the structural aspects of protein responsible for the diseases, (heart disease, Parkinson's and Haemolytic anaemia) those diseases which ar commonly found. Here our emphasis was to study the 3D structure of selected protein molecules, their backbone and their specific template which can give us the information of active site and binding sites available in the molecules after performing the method of HMM.

here we utilized the SpDbV application for 3D work on our molecules.

Related work

2. Methodology : In this work we tried to study protein structure prediction implementing the sequences of three different diseases, here the information was pulled out from the biological databanks and sequences where searched for similarity (E-value picture 1)

$$E = Kmn\, e^{-\lambda S}$$

Picture 1 Equation of E-Value

After aligning the sequences, there structured had been extracted and proceeded for the structure anaylsis in SpDbV, with the help of application we abled to get the template which can be fit into the Modelling process.

3. Spdbv structure of proteins And Result

1)Soy protein: (protein for Heart disease) =From the screening we get proper e-value in homo sapien is 0.0 and query sequence is >=200. Using spdvb software we study mutated sequence for drug designing.

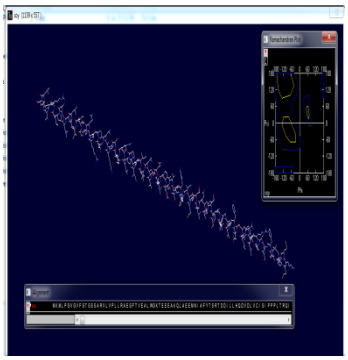

Figure 1

2)Alpha-synuclein(Parkinson'sDisease) from the screening we get proper e-value in homosapien is 4e-04 and query sequence is 40-50%.

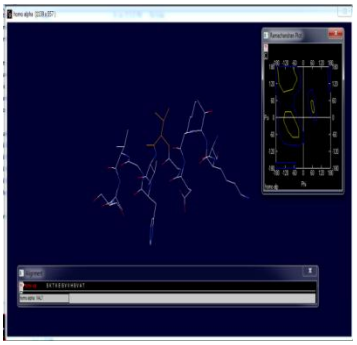

Figure 2

3)Haemoglobin (Haemolytic Anemia)

From the screening we get proper evalue in homosapien is 1e-95 and query sequence is >=200% . using spdvb software we study the mutated sequence for drug designing.

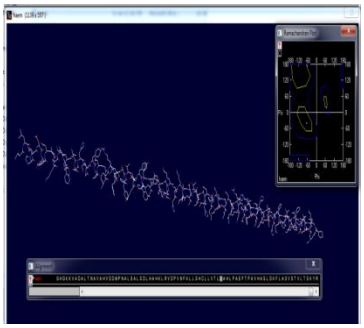

Figure 3

4. Conclusions

Proteins play important roles in various diseases. Through analyzing the properties and characteristics of protein we try to find their involvement in disease. Structural analysis of the proteins pave our ways to find solution to certain diseases .In order to analyze proteins which structures have not been determine yet, we use homology modeling to model proteins by using appropriate templates with the help of HMM

we will reveal the significance of the proteins in disease from their structural analysis.

5.Future Aspects

1.The predicted structures of our target proteins help us to analyze the significance of the proteins and its involvement in diseases. Thus we have better understanding of disease.
2.Structural bioinformatics can play a key role in structural based drug designing.
3. When a particular target is inaccessible to structural biology, a project may role on the use of a related protein for structure determinations. we can use surrogate proteins from another species or similar member of the gene family.

References

1)Brocchieri L, Karlin S (2005-06-10). "Protein length in eukaryotic and prokaryotic proteomes". Nucleic Acids Research 33 (10): 3390–3400. doi:10.1093/nar/gki615. PMC 1150220. PMID 15951512.

2)Marti-Renom, MA; Stuart, AC; Fiser, A; Sanchez, R; Melo, F; Sali, A. (2000). "Comparative protein structure modeling of genes and genomes". Annu Rev Biophys Biomol Struct 29: 291–325. doi:10.1146/annurev.biophys.29.1.291. PMID 10940251.

3)Chung SY, Subbiah S. (1996.) A structural explanation for the twilight zone of protein sequence homology. Structure 4: 1123–27. 4)Williamson AR (2000). "Creating a structural genomics consortium". Nat Struct Biol 7 (S7):95-108

5)Venclovas C, Margelevičius M (2005). "Comparative modeling in CASP6 using consensus approach to template selection, sequence-structure alignment, and structure assessment". Proteins 61 (S7): 99–105. doi:10.1002/prot.20725.

6)Dalal S, Balasubramanian S, Regan L. (1997). Transmuting alpha helices and beta sheets. Fold Des 2(5):R71-9