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Research Article

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Computational Method for Molecular Structure Prediction and Visualization of Target Protein Molecule

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ABSTRACT

In biological science the structure prediction and in silico analysis is basic technique to visualize the cell's molecules.In bioinformatics, software technology and sophisticated computer graphic program have been developed for visualization of three dimensional structures of biomolecules. These computerized generated graphics help to analyze and compare protein structures to gain insight to functions and properties of protein. In this present study molecular structures are being predicted with the help of molecular modeling and visualization tools. Computer visualization programs has feature like interactivity, which allows users to virtually manipulate the molecular structural images.

Keyword: *Molecular visualization, Structure Prediction, Secondary structure, Modeling, Computer tools.*

INTRODUCTION

Different types of bio molecules founds in living creatures, and they cannot be visualized directly[1-3]. Protein found abundantly in cells of organisms[4-5]. After experimentation, once a desired or target protein structure has been solved it has to be presented in a three dimensional view on the basis of the solved Cartesian coordinates[6-8]. Before computer software for visualization was developed, molecular structures were represented by physical model of metal wires, rods, and spheres like structures[9]. With the recent advances in development of computer hardware with higher graphical processing unit and software technology, sophisticated computer graphics program have been developed for visualizing and analysis of molecular structure[10-12]. This specialized computer software's are capable to rotate, zoom and manipulate the color image of target molecule[13-15]. Molecular visualization programs are graphical user interface and technically interactive[16]. Different types molecular structure can be predicted, depends on the capability and features of software[17-20]. Predicted structure manipulations can include changing the conformation of a structure by protein modeling or matching a ligand to an enzyme active site through docking exercises[20-21]. Different styles molecular structures are being predicted and shown in this study.

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MATERIAL AND METHOD

A. Amino acid sequence of Target protein
B. SWISS-MODEL Workspace
C. PDB file of target protein
D. Molecular visualizing programs:
1. RasMol
2. PyMOL

E. Image processing software

Retrieval of Amino acid sequence:

The amino acid sequence for target protein, human insulin was obtained with accession number **AAA59172.1** from NCBI server[22].

Preparing and Obtaining PDB file:

Amino acid sequence was subjected to modeling towards and alignment of target sequence with SWISS – MODEL WORKSPACE SERVER[23]. From automated mode sequence was aligned and target protein modeled file was obtained in PDB format.

Molecular structure prediction and visualization:

RasMol[24] and PyMOL[25] software used for molecular structure prediction of target molecular protein. Prepared protein file open and analyses for different structure prediction. Utilizing above software, clear colorful structure images in different form was obtained.

RESULT AND DISCUSSION

Molecular structure of target protein was predicted and visualized through PyMOL. Different type molecular structure were predicted in high quality color image form. Four type molecular structures are being predicted and visualized in this study, (A) Wireframes. (B) Balls and sticks. (C) Space-filling spheres. (D) Cartoon.

Predicted structure of insulin in Hexamer form, as target protein molecule shown in Figure 1. Figure 2 reveals the wireframes structure of target protein molecule. Figure 3 reveals Ball and stick structure. Figure 4 reveals the space-filling sphere structure and Figure 5 reveals the cartoon structure of target protein molecule.

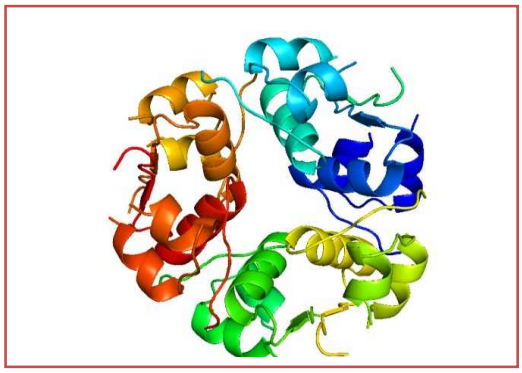

Fig. 1: Hexamer cartoon structure of Insulin.

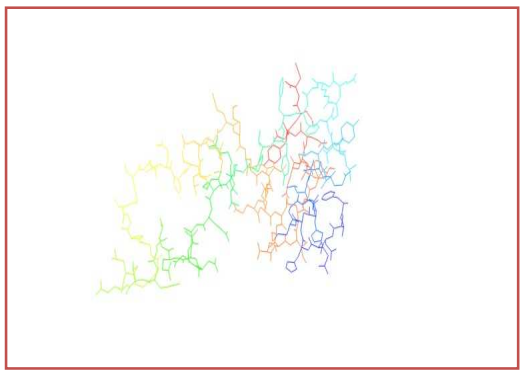

Fig. 2: Wireframe structure of Insulin.

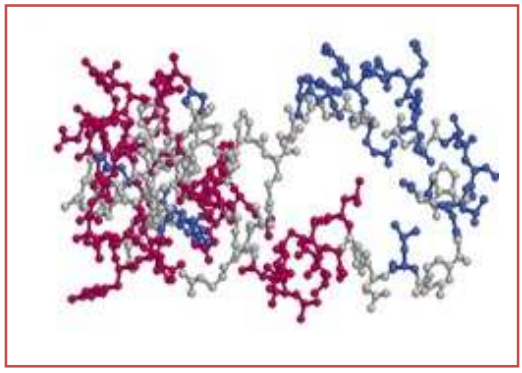

Fig. 3: Ball and Stick Structure of Insulin.

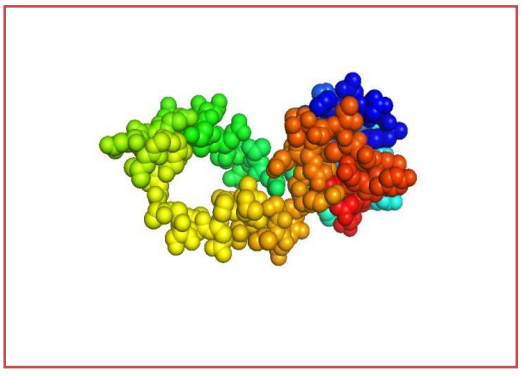

Fig. 4: Space-filling sphere structure of Insulin.

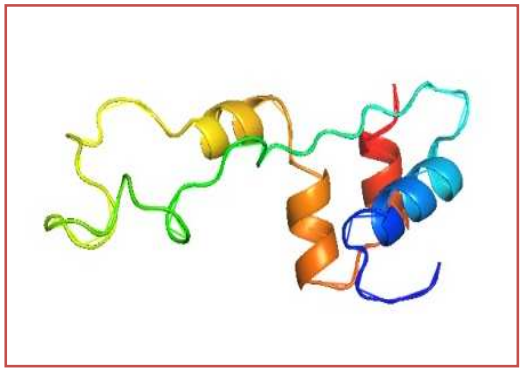

Fig. 5: Cartoon structure of Insulin.

CONCLUSION

Computational structural biology has made tremendous progress over last two decades in molecular prediction and visualization. Molecular structure prediction and visualization are required specialized computer software's and tools. Structure prediction and visualization provides specific structural information about molecule or protein virtually, real time on computer. Molecular visualization allow user to rotate, flip, and manipulate virtual molecular models of chemicals and macromolecules. Molecular structure prediction and visualization are key step in drug discovery and molecular docking.

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