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Contmann: A Tool to Calculate Contact Distances Between Amino Acid and Mannose Using Protein Data Bank File at Distance Cutoff

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ABSTRACT

Protein function depends on interaction with their ligands and mannose is one of the important ligands for understanding glycoprotein, so it is often required to calculate the binding site residues in protein at different distance threshold from PDB file. To study particular protein chain and its interaction with mannose in complex form, researchers have to parse the output of different available tools or databases for binding-site residues. Here we have developed a tool for calculating amino acid contact distances in proteins at different distance threshold using PDB file. ContMann can quickly find all binding-site residues in the protein by calculating distances from its coordinate present in pdb file by selecting the different distance threshold, Additionally, it can also generate atomic details of contacts including distances of binding-site residue. ContMann tool is available at: http://procarb.org/procarbdb/cfind-contact2.html

KEY WORDS: PROTEIN FUNCTION DEPENDS, CONTACTS INCLUDING DISTANCES..

INTRODUCTION

The proteins function depends on interaction with their ligands, among ligands Mannose is very important (Turner MW, 2003, Ng KK, 2002). Therefore, identifying amino acid contacts is important for understanding the glycoproteins. In order to understand the interactions calculating the amino acid contacts at different distance thresholds required (Kenneth, 2002). Binding site residues of proteins can also be identified from databases (Desaphy 2015), visualization tools (Jendele 2019), or many other web servers developed earlier (Jendele 2019, Angles 2020), but this becomes overwhelmingly imposing when a large set of proteins have to be analysed.

With the help of this tool, user can get the binding residue by after uploading PDB file. Additionally, it can also generate atomic details of contacts including distances of binding-site residue from PDB structures. Protein Data Bank (PDB) is repository of for 3D structures of biological macromolecules which has coordinates of its atoms (Kayikci 2018; Berman 2003), using these coordinates of two atoms, this tool can compute the distance between them.

A residue is defined as a binding residue if the distance between atoms of the interacting partner is less than a certain distance cut off (Eyal 2001). Upon uploading the protein mannose 3D-structure file of interest and option selected for distance threshold by user, ContMann searches the PDB file for the protein chains, Ligand chain of interest and the number of protein models (if multi model protein). If more than one model is present,

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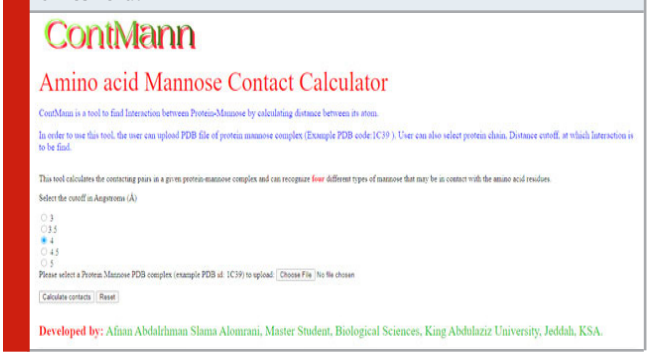
ContMann gives option to select and parse the desired model present in the uploaded Protein Data Bank (PDB) file. Then ContMann calculates the distance between selected protein chain residue atoms and interacting partner atoms, and when this distance falls below or equal to the selected distance threshold, this residue is considered as binding residue. The overall description is illustrated at home page (Figure 1).

Web Interface: Web interface of current version of ContMann developed using HTML, JavaScript and CGI-PERL scripting language. It has home page where description about this tool mentioned, uploading pdb file option and submit button provided, here user can also select distance threshold in angstrom (Figure-1)

Figure 1: Screen shot of ContMann Home page. From this home page user can upload PDB file and select distance threshold.



Program input: The input to the ContMann is a protein 3D coordinate PDB file, modeled protein or a docked complex file. The user can select provided distance threshold also (figure 1).

Figure 2: Screen shot of output page. Here user can find the interaction residues with its atom, distances in angstrom and summary of Amino acid contact with mannose.

Program output: At the top of the program's result page (figure 2), the uploaded file name and distance threshold selected for the calculations are displayed. The calculated distance between the two atoms, its residue, protein chain and the interacting atoms is displayed in a tabular form (figure2). The page summary section has total number of contacts at the end of page. First five column has distance, residue, position, atom and chain of protein and last 3 column has ligand three letter code, atom and chain of ligand. At the end of output summary of binding residue also mentioned.

Proteins are complex and have different conformations, that are often related to the protein function (Karplus 2005). Mannose binding proteins act as receptors and take part in innate immunity, human mannose-binding protein also has role in first line host defense (Ezekowitz 2003; Turner 2003). Identification and analysis of binding sites of protein with mannose are important and needful.

CONCLUSION

The developed tool will be useful for the identification and analysis of binding sites residue of protein from 3D-structure PDB file of protein mannose complex at different distance threshold. Although, in current version only one pdb file can be uploaded but it will be upgraded for batch file, so user can upload list of files.

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