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PREDICTION OF LIGAND BINDING SITE IN GLOBULAR PROTEINS

R.Senthil, S.Sathish, J.Jannet Vennila and E.Rajasekaran*
Department of Bioinformatics
School of Biotechnology and Health Science, Karunya University, Coimbatore – 641114
*Correspondence (sekaran@karunya.edu)

ABSTRACT

Prediction of protein's active site from three dimensional structure is first and foremost step for drug discovery. There are several tools available for this purpose. It use different principles and methodologies. But the fact is that hydrophobic interaction is the dominant force that determines this site. Ultimately, the carbon becomes important at the active site as it is the one only element contributes towards this interaction. We have developed a tool based on this carbon distribution in proteins that is capable of predicting the binding site. A comparative analysis of our result with known pdbsum results is presented.

Keywords: Carbon distribution, active site, binding site, hydrophobicity, sequence analysis, pdbsum.

INTRODUCTION

Active sites in proteins are three dimensional substructures that cause them to perform their function. The problems of finding substructures in a protein that are active sites of protein which helps to solve the functional problem. The protein active site has several important applications in biological sciences such as drug design, genetic engineering, and diagnostic tools for analysis of genetically engineered pathogens. In recent years the prediction of protein 3D structures growing rapidly in several new ways with little or no functional information. So is the case with identification of functional sites. For solving this problem of functional site identification as the case like active site, binding site and protein-protein interaction regions identification (Senthil and Rajasekaran**,** 2010), this require proper understanding of proteins in water. Several methods and tools are used for this purpose but with less accuracy. Hydrophobicity plays major role in molecular association in water. Carbon is single most element contribute towards this (Rajasekaran *et al*., 2009; Senthil and Rajasekaran**,** 2009**;** Senthil and Rajasekaran**,** 2010). So a tool for finding binding site based on carbon distribution is required to be developed.

METHODOLOGY

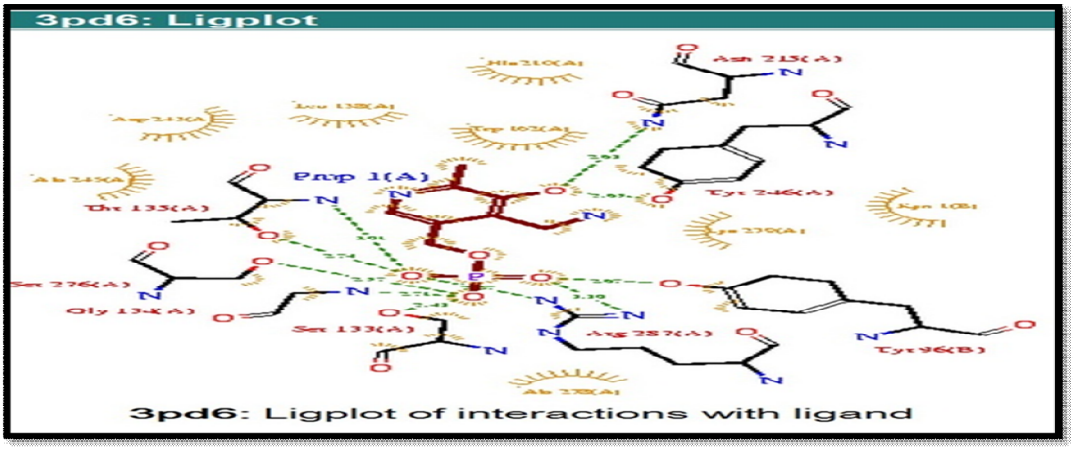
For this study we used the known protein mouse mitochondrial aspartate aminotransferase, a newly identified kynurenine aminotransferase-IV (PDB ID: 3PD6). The home made active site finding tool based on carbon content (Rajasekaran and Vijayasarathy, 2011) is used to find active site or ligand binding site of the protein. It scans the protein sequence for carbon content. Based on carbon content, a portion of sequence which has more than 31.45% of carbon is considered as active sites (Senthil and Rajasekaran**,** 2009). The online tool PDBSUM from EBI is used to predict the active site for comparison. The results are plotted as shown in the picture

RESULTS AND DISCUSSION

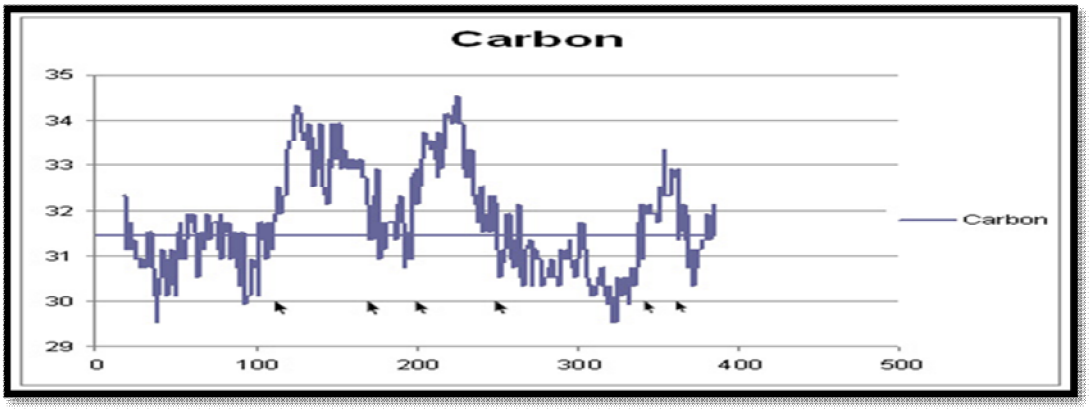
The active site identifications from sequence information are reported here. A known case of protein (PDB id: 3pd6) from pdbsum of EBI is taken for study. The pdbsum reports that the residues, His210, Asn215, Leu138, Asp243, Trp162, Tyr246, Ala245, Ser276 and Ser133 are in the active site. Our program predicts the regions at which these residues belong to are carbon rich region that can be noted using arrows. More over it is not the single residues responsible at the active site but several of them. The residues Arg287, Lys279, Ser276 and Ala278 are also in the active site. This

occurs at the hydrophilic regions. This may be the other atoms of the ligand binds to this region. Our program can be accessed online (www.rajasekaran.net.in). A comparative analysis of our result with pdbsum is shown in figures.

PDBSUM: (3PD6 Ligplot)



CARBON PLOT FOR 3PD6:



CONCLUSION

The prediction of active sites or binding sites from sequence information is reported here. Carbon rich regions are considered as binding sites. Our program, based on carbon content is able to identify these binding sites. The results are compared with PDBSUM and result.

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