IDENTIFICATION AND CHARACTERIZATION OF GENES CONFERRING INSECT RESISTANCE BY IN SILICO AND BIOINFORMATIC METHODS

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Abstract: From several years entomological and plant pest interactions research is focusing on protease inhibitors (PIs) based strategies for controlling insect pests. Present review signifies the importance of in silico analysis of interactions between insect gut proteases with PIs and provides the information of tools and techniques such as molecular docking and molecular dynamics required for analysis. In silico prediction of insect gut protease and PIs interactions could provide significant information for identification and development of novel promising PI candidate for the transgenic approach.

Keywords: Molecular docking, Molecular dynamics, Plant Protease Inhibitor.

INTRODUCTION

Protein-protein interactions are involved in most biological processes and are important targets for drug design. Over the past decade, there has been increased interest in the design of small molecules that mimic functional epitopes of protein inhibitors. The amalgamation of computational and experimental approach has been of great value in the identification and development of novel promising results. In silico prediction of functional regions on protein surfaces, i.e. sites of interaction with DNA, ligands, substrates and other proteins, is of utmost importance in various applications in the emerging fields of proteomics and structural genomics [1]. Detection of the amino acid positions that are essential for activities, such as catalysis, protein-protein interactions or protein–ligands interactions, is a critical step in the study of the biological function of proteins [2]. Determination of protein structure by the experimental method has often limitations. For that need, computational approach such as molecular docking plays a vital role. Protein-protein interaction has considerable attention in drug discovery [3].

MATERIALS AND METHODS

In silico prediction of insect gut protease and PIs interactions could provide significant information for identification and development of novel promising PI candidate for the transgenic approach. This will also minimize the cost and period of in vitro screening of PIs.

RESULTS AND DISCUSSION

Figure 1 depicts a possible mechanism of virtual screening of fragment library. An inhibitor molecule is one which has the ability to bind to the catalytic site of the enzyme. The inhibitor may be developed as libraries (collection) of many potential molecules (short fragments) or individual ligands. Natural compound libraries are most widely used for screening with target catalytic site. Virtual screening is a docking approach used to computationally screen large libraries of chemical compounds (inhibitors). The expensive high-performance computation platforms have changed the way to performing virtual screening which gives detailed and relevant biological data.

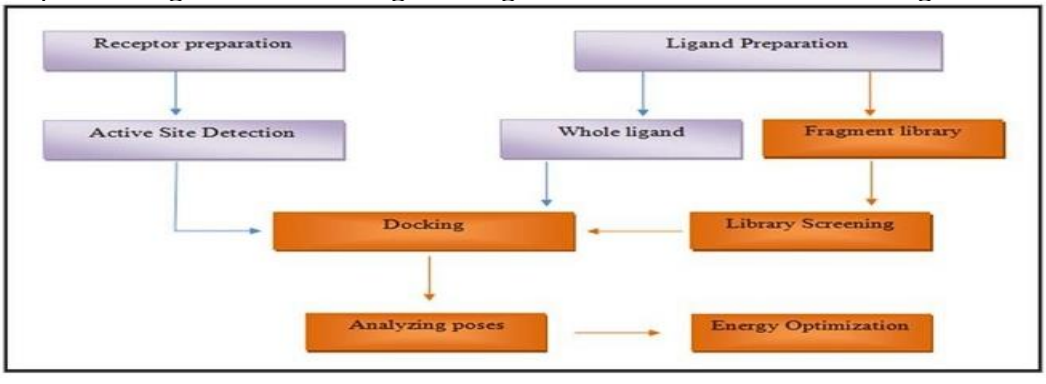

Figure 1: Possible mechanism of virtual screening of fragment library

The molecular mechanics or molecular dynamics allow prediction of equilibrium geometries and energies between different molecules. Molecular mechanics results in the geometry of the motionless molecule. Dynamics studies often important to understand the protein folding and unfolding [4]. Misfolding will lead to malfunctioning such as causing disease, interruptions in signal transduction and genetically changes in evolution time. Its more often need to study how the movements affect the function of the protein and how their dynamics are related to the 3D folding. Molecular dynamics gives details change in individual particle motion respect with time. Computational evolution provides significant developments in molecular dynamics studies. Protein-protein interaction refers to a physical binding between two or more proteins. Such a physical interaction can be categorized based on the composition of the complex, the function of the complex versus that of a monomer, the binding affinity of subunits in the complex, the duration of the complex formation, or interactions between specific functional groups. Protein-protein interactions in plant-arthropod interactions can be studied by above mentioned computational approaches to design competent strategies against insect pests.

CONCLUSION

Advances in computational biology tools led to the foundation to in silico study of protein-protein interactions prior to in vitro screening of target molecules. These approaches could be implemented to design lead/inhibitor molecule against digestive proteases of insect pests to design capable strategies against insect pests.

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