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Short Communication

IN SILICO HOMOLOGY MODELING OF SYSTEMIN RECEPTOR SR160 - THERAPEUTICAL TARGET FOR THE INDUCTION OF THE CELLULAR DEFENSIVE GENE

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ABSTRACT

Systemin receptor (SR160) is a plasma membrane bound receptor protein, work as key regulatory signals for the activation of defensive mechanism in tomato plants. It has been confirmed that systemin is plant peptide hormone containing 18 amino acids, binds with its known receptor SR160 to activate the downstream cascade pathway for the activation of defensive genes in tomato. 3D structure of SR160 was not available so homology modeling was preferred to generate the good quality model. For the verification of the model procheck was used. The predicted model can be for the prediction of binding interaction and structure-based drug designing.

Keywords: Systemin, Systemin receptor SR160, 3D structure, Homology modeling, Procheck.

1. INTRODUCTION

Systemin is an 18-amino acid plant peptide hormone that can coordinate humoral and cellular immune responses. By releasing systemin itself from substrate prosystemin, binding systemin to its membrane protein Systemin Receptor (SYR), as well as transporting deep signalling molecules such as jasmonic acid, prosystemine messenger RNA, and polycyclic aromatic hydrocarbons, the classical system activates the systemic signalling pathway. We present new information that the platform's disturbed structure, experimental processing, and protein secretion contribute to system-mediated signal transduction in plant defence [1]. Protein-protein interactions are crucial at almost all levels of cell function. Flexible proteins and peptides account for approximately 40% of all protein-protein interactions [2], when it binds to protein receptors, it folds. Peptide deficiency is referred to as intrinsically stable secondary disordered tertiary structure protein (IDP) deficiency [3]. It plays an important role in cellular processes, regulation, and control of biosynthetic systems. It is related to the activation of genes that control the functions of living cells in plants, either directly or indirectly. Disordered peptide fragments interact with various proteins in multiple pathways and are thus linked to a variety of diseases. Systemin is a type of PID found in tomato leaves that contains 18 amino acid sequences and is derived from the prohormone precursor prosystemine. In 1991, the compound was isolated from the plant leaves of *Solanum lycopersicum*, also known as tomato [5]. Systemin hormones have been identified as signals that initiate the systemic wound response. Systemin binds to its SR160 receptor, triggering an intracellular signal cascade that activates protective genes [4] (Fig. 1).

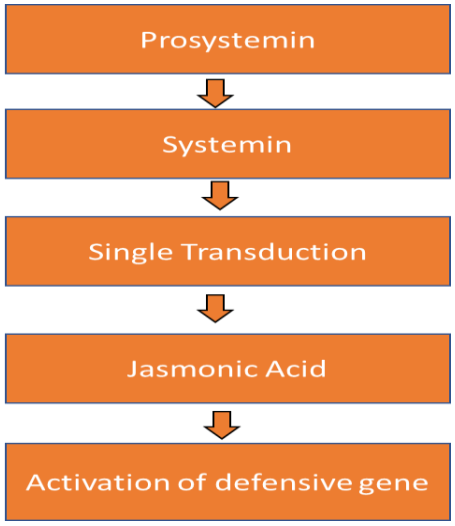

Fig. 1: Activation steps of defense genes in the intracellular pathways of the tomato plant

The tomato SR160 system protein receptor (wild tomato) is said to be a member of the leucine-rich repeat receptor (LRR) family of kinases and is related to

Arabidopsis thaliana's brassinolide BRI1 receptor kinase, Sequence homology in kinase and domain site regions. Systemin signalling activates the 2nd regulator of JA (jasmonic acid) via SR160, which in turn activates defence gene expression, thus identifying it as the systemin receptor that activates the cascade pathway [6]. However, no experimental studies have been conducted to determine how system proteins bind to SR160.

2. MATERIAL AND METHODS

2.1. Sequence Retrieval

Data from experiments Sequence alignment and structure prediction The SR160 query sequence (*Solanum lycopersicum*) amino acid sequence was obtained from the NCBI database (accession number: Q8GUQ5) (https://www.ncbi.nlm.nih.gov/). Used the Basic Local Alignment Search Tool 8 (BLAST) to find the perfect match structure template. Brassinosteroid LRR receptor kinase PDB ID: Q8L899 has 90 percent similarity and 1.90 resolution, making it an excellent template. Modeller 9.179 was used to create the 3D structure.

2.2. 2-Dimensionalprotein Structure Validation

The derived protein model's quality is assessed using *in silico* tools such as PROCHECK and protein structure analysis (ProSA) [8, 9]. PROCHECK is a program that depends on Ramachandran diagrams for structural confirmation and calculates the stereochemical geometry of the model. In addition, ProSA is used to check standard parameter (energy) and compare them with a huge number of known protein structures of same size [10]. The configuration file is written to the SR160 configuration file, which can be utilized as input to a graphics program (tool is GNUPLOT).

2.3. Accessible surface area (ASA) analysis

VADAR (http://vadar.wishartlab.com/) server 34 merges over 15 algorithms and programmes for evaluating peptide and protein structures based on PDB coordinate data.

3. RESULTS AND DISCUSSION

In this experiment, we used a homology model to evaluate the 3-Dimensional structure of SR160 to explore the binding and interaction of Systemin and SR160. The key role in initiating this pathway involves the release compound of linolenic acid from the mitochondrial membrane, which is then converted to jasmonic acid. It may activate defence genes in tomato plants (11). We obtained the fasta sequence of SR160 from the NCBI database research to defend against predators by synthesizing defensive chemicals (Fig.2).

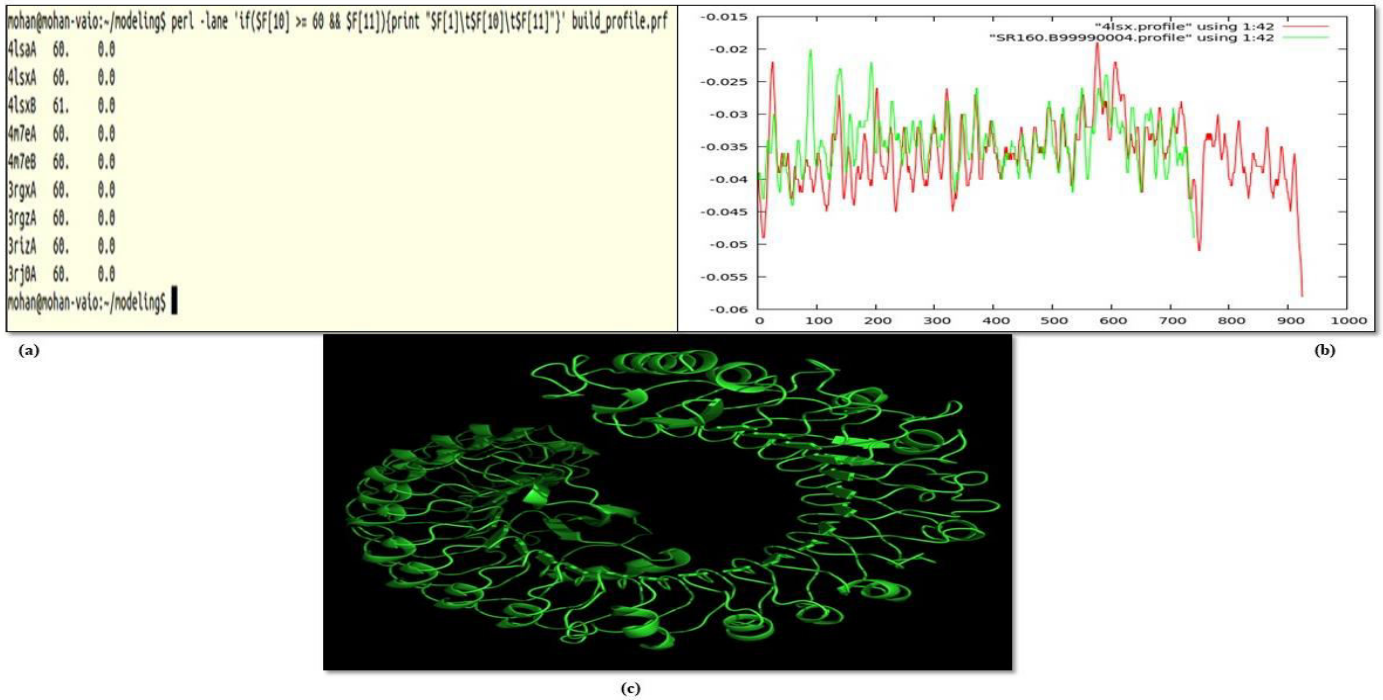

Fig. 2: (a) The database evaluates model.py can be used to create a model's pseudo-energy profile.(b) A comparative analysis of the model's (red) and template's (green) pseudo-energy statuses(c) Homology model of SR160

Systemin is an 18-amino acid polypeptide hormone in plants that is responsible for activating defence genes. Systemin is an 18-amino acid polypeptide hormone found in plants that activates defence genes. Systemin is distributed in tomato leaf wounds and binds to the cellular receptors SR160 to perform gene activation downstream. The amino acid sequences of system proteins are all stable, which is significant for the maximum oxidation of protease inhibitor of specific genes. According to their binding protein interactions, the amino acids (AA) near the COOH end are accountable for the protein function, while the AA near the NH end are responsible for interacting with the binding site. It is not clear how systemin binds to its SR160 receptor and what is the functional structure of its natural complex.

Table 1: Successfully produced models

Different File	Molpdf file	DOPE scoringvalue	GA341 scoringvalue
SR160.B99990001.pdb	5355.24414	-84000.07812	1.00000
SR160.B99990002.pdb	5433.86914	-82970.92969	1.00000
SR160.B99990003.pdb	5381.18994	-83419.46094	1.00000
SR160.B99990004.pdb	5429.87793	-84220.21094	1.00000
SR160.B99990005.pdb	5474.54053	-83519.13281	1.00000
SR160.B99990001.pdb	5355.24414	-84000.07812	1.00000
Total CPU time [seconds]		: 343.71	

4. CONCLUSION

The 3-dimensional structure of SR160 was generated which is useful to study protein-ligand interactions to develop drugs to target the mutated protein- a target in AD. The template SR160 was chosen which has 86% identity score with query sequence. The models of SR160were generated using the Modeller 9.20, modal quality is evaluated by computational analysis such as PROCHECK and Protein Structural Analysis (ProSA which clearly shows the good quality of the obtained models. Future perspectives will be to study the dynamics of each atom present in the structure and the other stimulations can also be considered. The mode of inhibitions can be studied with the predicted models using *In silico* approach as it be the therapeutic target for the intracellular signalling molecules interaction leading to protective gene activation. Few other mutated models can also be predicted specifically and docked with the ligands to check the activity of certain drugs.

Conflict of interest

None declared

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