IN SILICO MODELLING AND MOLECULAR INTERACTION OF ELONGATION FACTOR RECEPTOR WITH PATHOGENIC ELONGATION FACTOR TU 18

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ABSTRACT

Plants depend entirely on innate immunity system to protect them from various pathogenic bacteria, fungi, and viruses. The first layer defense mechanism is named as Pattern-triggered immunity (PTI) system. It is activated by Pathogen-associated molecular pattern (PAMP) of the host plant by Pattern recognition receptor (PRR) with the aid of co-receptor. Elongation factor receptor (EFR), which is also known as PRR, is one of the most recognized receptor used to protect against disease in Brassica species. Although research on transgenic approach and wet labs experiments have been carried out to analyse the EFR model, but the full ectodomain interactions of EFR with PAMP elf18 protein and co-receptor Brassinosteroid Insensitive 1-associated receptor kinases (BAK1) protein through *in silico* has not been accomplished yet. The purpose of this study was to determine the interaction of EFR protein with elf18 protein through *in silico* analysis approach. In this study, PRR EFR protein and PAMP elf18 protein was constructed by homology modelling using HHpred Modeller, followed by docking and molecular dynamics (MD) simulation of EFR protein and elf18 protein with co-receptor BAK1 protein (PDB:3UIM) and apo BAK1 (PDB ID:3ULZ) as model for mutant protein using ZDOCK 3.0.2 server and GROMACS 5.0.4 respectively. Finally, superimposition was done between EFR-elf18-BAK1 complex with existed FLS2-flg22-BAK1 crystal structure. Modelling results showed that multiple template modelling (MTM) generated best models compared to single template modelling (STM) due to their best quality of the protein structure obtained by HHpred Modeller generate best validation results of 71.123 ERRAT, 95.67% Verify3D and 92.8% in favoured region of Ramachandran Plot. Docking results showed that the complex interaction of BAK1 protein and elf18 protein binds at the concave surface of Leucine-Rich-Repeat (LRR) EFR, compatible with the existed FLS2 complex binding interactions. For the EFR-elf18-BAK1 (normal) complex, about 20 hydrogen bonds were sustained which is higher compared to EFR-elf18-BAK1 (mutated) complex that only sustained 16 hydrogen bonds, proved that the mutated protein have less interaction after simulation. After 50ns MD Simulation, the results showed that all the docked complexes has significant reduction of H-bonds. For EFR-elf18-BAK1 docked complex, H-bond between EFR protein and BAK1 protein reduced from 45 to 22, and H-bond between elf18 protein and BAK1 protein were reduced from 9 to 0 which caused by the conformational changes of the proteins during simulation. This study helps to understand the Brassica disease in detail and contribute significantly to early event of Pattern Triggered Immunity mechanism of EFR-elf18-BAK1 protein complex.

ABSTRAK

Tumbuhan bergantung sepenuhnya pada sistem keimunan inat untuk mempertahankan diri dari serangan bakteria, kulat dan virus.Lapisan pertahanan pertama adalah dikenali sebagai sistem imuniti cetusan corak (PTI). Sistem tersebut diaktifkan melalui mikroorganisma tanggapan relatif patogen (PAMP) oleh reseptor pengesanan corak (PRR) tumbuhan perumah dan protin ko-reseptor. Reseptor faktor pemanjangan (EFR) adalah antara reseptor pengesanan corak (PRR) yang merupakan reseptor yang paling dikenali untuk melindungi daripada penyakit dalam spesies Brassica.Walaupun beberapa kajian melalui pendekatan transgenik dan eksperimen makmal telah dijalankan untuk menganalisis model EFR, namun interaksi penuh antara EFR dengan protin elf18 dan protin ko-reseptor BAK1 dalam kajian *in silico* masih belum dilakukan. Tujuan kajian ini dijalankan adalah untuk mengkaji hubungan interaksi di antara protin EFR dengan protin elf18 melalui pendekatan secara *in silico* . Dalam kajian ini, (PRR) protin EFR dan PAMP protin elf18 telah dibina melalui pemodelan homologi menggunakan HHpred Modeller diikuti proses mengedok menggunakan perisian Z-dock dan simulasi dinamik, GROMACS bersama protin ko-reseptor BAK1 (PDB: 3UIM) dan mutannya yang dikenali sebagai apo (PDB: 3ULZ). Akhir sekali, hasil keputusan dok iaitu komplek EFR-ef18-BAK1 dibandingkan dengan struktur kristal yang telah sedia ada iaitu FLS2-flg22-BAK1. Keputusan pemodelan menunjukkan bahawa templat tunggal tidak mampu memperoleh struktur model yang berkualiti dan hanya perisian Modeller yang berhubung dengan HHpred mampu memberi keputusan model yang terbaik iaitu sebanyak 71.123 ERRAT, 95.67% nilai Verify 3D and 92.8% asid amino di dalam kawasan yang dibenarkan dalam plot Ramachandran. Keputusan analisis menunjukkan mekanisma pelekatan oleh dok dengan protin BAK1 dan protin elf18 menghasilkan bentuk permukaan cekung mengikat di sebelah sisi EFR LRR yang lebih serasi dengan komplek yang sedia ada iaitu FLS2. Bilangan ikatan hidrogen adalah tinggi (20) bagi komplek EFR-elf18-BAK1 (normal) berbanding komplek EFR-elf18-BAK1 (bermutasi) (16) di mana ini membuktikan kesan mutasi yang memberi interaksi yang kurang selepas proses simulasi. Keputusan simulasi dinamik pada 50ns menunjukkan kehilangan ikatan hidrogen pada kesemua struktur yang telah didok. Bagi dok kompleks EFR-elf18-BAK1, ikatan hidrogen antara protin EFR dan protin BAK1 berkurang daripada 45 kepada 22, dan ikatan hidrogen antara protin elf18 dan protin BAK1 berkurang daripada 9 kepada 0 yang mungkin berpunca daripada perubahan konformasi protin semasa proses simulasi dinamik. Hasil kajian ini membantu untuk memahami penyakit dalam tumbuhan Brassica dengan terperinci dan mungkin menyumbang kepada pemahaman peristiwa awal PTI oleh kompleks protin EFR-elf18-BAK1.

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LIST OF ABBREVIATIONS

BAK1	-	BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1
EFR	-	Elongation Factor Receptor
EF-Tu	-	Elongation Factor Thermo unstable
ETI	-	Effector Triggered Immunity
GROMACS	-	Groningen Machine for Chemical Simulations
H-bond	-	Hydrogen Bond
JM	-	Juxtamembrane Domain
LRR-RK	-	Leucine Rich Repeat Receptor Kinases
MD	-	Molecular Dynamics
PAMP	-	Pathogen Associated Molecular Pattern
PDB	-	Protein Data Bank
PRR	-	Pattern Recognition Receptor
PTI	-	Pattern Triggered Immunity
Rg	-	Radius of Gyration
RMSD	-	Root Means Square Deviation
RMSF	-	Root Means Square Fluctuations
SERK	-	Somatic Embryogenesis Receptor Kinase
TM	-	Transmembrane Domain

LIST OF SYMBOLS

%	-	Percentage
Aº	-	Angstrom
α	-	Alpha
β	-	Beta
ns	-	Nano second
ps	-	Pico second
nm	-	Nano meter

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CHAPTER 1

INTRODUCTION

1.1 Background of study

Arabidopsis plant consists of various disease resistances majorly in *Brassica* species. *Brassica* plant species such as Cabbage (*Brassica oleracea* var. *capitata* L.) is one of the main vegetables consumed in Malaysia as fresh market vegetable and also eaten fresh in food consumption such as coleslaw, sauerkraut and cabbage roll. It has contributed to greatest production in many parts of Malaysia, especially in Cameron Highland with 92% of total cabbage production annually. However, it also causes 11% of crop loss each year since 1925 due to pest infestation (Mazlan & Mumford, 2005). The *Brassica* species mainly affected by diseases such as *Xanthomonas campestris* and *Plamodiospora brassicae* causes by the most prominent insect pest, *Plutella xylostella.* There is a lot of research has been already done to control the disease such as transgenic crops as well as the usage of the biological insecticide and insect-resistant genetically modified crop which is ineffective due to some of the factors such as short-lived of plant species, non-environmental friendly and highly cost (Bravo Alejandro & Gill Sarjeet, 2008).

Many research recently focused on in silico analysis study where all data of biological experiments are being carried out entirely using computer. Pattern recognition receptor (PRR) plays an important role in in silico study for rapid detection of potential danger caused by pests and microbes by pathogen-associated molecular pattern (PAMP). *Arabidopsis thaliana* is currently used to analyse the microbial-plant interaction through in silico analysis (Bigeard *et al.*, 2015; Kunze, 2004). From *Arabidopsis* plant, many PRR have their own specific binding with PAMP. Flagellin Sensitive2 (FLS2) and Elongation factor receptor (EFR) are the most-characterized membrane protein used for in silico study. However, the overall structure of protein complex FLS2LRR-flg22-BAK1LRR has already been analyzed

through in silico binding mechanism (Sun *et al.*, 2013), in which LRR indicated as leucine rich repeat domain.

The perception of bacterial elongation factor Tu (EF-Tu) by Elongation factor receptor (EFR) protein explains the well-studied PAMP/PRR pair specifically for *Arabidopsis* plant disease (Roux *et al*., 2011; Sato *et al*., 2000). Elongation factor Tu (EF-Tu) is the most abundant bacterial protein that acts as a pathogen-associated molecular pattern (PAMP). *Arabidopsis* plants recognize the N terminus of the protein comprises the first 18 amino acids of elf18 as it is fully active in defence responses (Albert *et al*., 2010). Additionally, the co-receptor such as Brassinosteroid Insensitive 1-associated receptor kinases (BAK1) protein and related somatic embryogenesis receptor kinase (SERK) protein helps to regulate and activate the immune response (Newman, Sundelin, Nielsen, & Erbs, 2013).

Previous research on transgenic expressions of LRR-RK EFR protein with different receptor protein of Flagellin Sensitive2 (FLS2) has been carried out through experiments such as binding assay, co-immunoprecipation, conservation mapping and others. Although most of PRR/PAMP have already been identified, however the full ectodomain analysis of EFR protein and its interaction with PAMP has not been carried out yet. Therefore, this current study attempts to interact LRR domain of EFR protein with elf18 protein and co-receptor BAK1 protein. This study significantly helps to analyse the brassica disease in detail and the interaction between EFR and elf18 in PTI system. Consequently, through the interaction, the similarity and differences with the existed complexes of FLS2-flg22-BAK1 is analyse through in silico analysis using bioinformatics approach.

1.2 Problem statement

The potential danger caused by insect pest, *Plutella xylostella* trigger the *Arabidopsis* plant disease and crop loss in *Brassica* species especially in cabbage. EFR is the most-characterized membrane protein, that has specific ectodomain

binding towards elf18 protein is used for in silico study to control the disease. When the pathogen attacked the plasma membrane, EFR protein will recognise the conserved PAMP and undergo downstream activities (Bigeard *et al*., 2015; Che, 2017). Recent research has been done in many wet lab experiments on transpecies transfer of LRR-RK EFR protein and different PRR to test the effectiveness of different plant species. Previous research has demonstrated co-immunoprecipitation experiments through *in-vivo* to test the ability of transgenic expressions of EFR protein and Flagellin Sensitive2 (FLS2) receptor with somatic embryogenesis receptor kinase (SERK) co-receptor in tobacco and tomato (Helft *et al*., 2011; Roux *et al.*, 2011)**.** Recent research also proved through conservation mapping method to predict suitable functional sites where it has been demonstrated through LRR domain of EFR protein and FLS2 receptor to test the resistance on bacteria *Ralstonia solanacearum* and *Xanthomonas campestris* pv. *Vesicatoria* (Helft *et al.*, 2011). However, the transgenic plants expressing EFR protein causes wilting symptoms. Moreover, chimeric receptor of FLS2 substitute with parts of EFR, which tested for functionality of ligand-binding-elf18 tobacco and tomato. Nevertheless, this research causes incompatible at the swap site and exchange of the LRR subdomain. Thus, due to the factors such as short-lived of plants because of high pressure of Bt Cry toxin, high cost and incompatible of swap site of protein domains, the previous research is considered ineffective. Thus, the current study proposed to investigate the random interaction of PRR of full EFR protein domain, without transpecies transfer of different receptor with elf18 and co-receptor BAK1 protein through in silico analysis approach by using various bioinformatics tool. This study concurrently helps to broaden the scope and increase the performance of the plant rather than experimenting using the same mainstream wet lab experiments.

1.3 Research Aim and Objectives

The overall aim of this research project is to understand the pattern-triggered plant immunity system to control disease in *Brassica* species mediated by EFR protein as pattern recognition receptor through in silico analysis study. The objectives of this research project are:

1. To evaluate structure reliability of single template models and multiple template models of PRR EFR protein and PAMP elf18 protein through structure validation analysis.
2. To determine random molecular interaction of complex of plant PRR EFR protein with PAMP elf18 protein through docking using ZDOCK 3.0.2 server.
3. To determine molecular interaction of complexes of plant PRR EFR protein and PAMP elf18 protein with co-receptor BAK1 protein through docking.
4. To determine structure stability interaction of docked complexes between PRR EFR protein and PAMP elf18 protein, together with the co-receptor BAK1 protein through molecular dynamics simulation.

1.4 Scope and Limitations of the Study

In the beginning of this study, initially the PRR EFR protein and PAMP elf18 protein was modelled using different tools, in which the amino acid sequence based analysis of EFR through multiple sequence alignment was done for EFR protein with its different template proteins. The homology modelling have been constructed to model the 3D structure of EFR protein and the final structure selected based on structure validation percentage using ERRAT, Verify3D and Ramachandran Plot. Following that, the random molecular interaction of PRR EFR protein, PAMP elf18 protein and co-receptor BAK1 protein was done by using ZDOCK 3.0.2 server. Then, molecular dynamics simulation was done to analyse the conformational changes of the proteins and stability interactions using GROMACS 5.0.4, which generated results in root means square deviation (RMSD), root means square fluctuations (RMSF) and radius of gyration (Rg) graphs. According to these measurement and other binding analysis measurements provided in methodology section, the results were assessed and discussed. For the binding interaction analysis, only LRR domain of EFR protein was taken into consideration since the mechanism happens outside membrane (R. Gupta & Bent, 2011).

The significant limitation for this study was that there is no research previously done for the in silico analysis study of EFR protein and interaction with its PAMP. Although EFR protein has been model previously, there is no reference on such interaction to PAMP elf18 protein as well for md simulation of pattern triggered immunity approach. The reference structure was only limited to FLS2 crystal structure having PDB ID of 4m8A, FLS2 complex as PRR with its PAMP flg22 and BAK1 as co-receptor which share similar co-receptor with EFR protein complex (Koller & Bent, 2014).

Another limitation of this study is that since this project mainly use online servers to accomplish work in order to model a protein, for the interaction and for simulation of protein. Moreover, not many free online modelling server could able to model full EFR protein together with all domains, thus separation of each domain has been done and has been model individually (Buenavista *et al*., 2012). As well for free docking tools, ZDOCK 3.0.2 was the most suitable to generate interaction between two or more different proteins compared to AutoDock 4.2.

1.5 Significance of study

The study of pattern-triggered immunity (PTI) system is important in order to understand the stages in plant defense mechanism in detail. Besides, PRR EFR is an important protein receptor in controlling major disease in *Brassica* species especially cabbage. Therefore, in silico study of EFR protein interact with PAMP elf18 protein and co-receptor BAK1 protein through proper modelling and molecular dynamics approach will significantly contributes knowledge to understand the plant defense mechanism.

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LIST OF PUBLICATIONS

1. Shivaranjini, G., Danian, A.F.A., & Hamdan, S. (2019). In-Silico Modelling of Pattern Recognition Receptor EFR and Molecular Interaction with Pathogen Associated Molecular Pattern elf18. *Proceedings of the 3rd International Conference On Social Science, Humanities and Technology (ICSHT 2019)*. 26-27 January 2019. Bayview Beach Resort, Penang. ISBN: 978-9672245-07-0.