Predicted of isoflavone reductase protein from oil palm and date palm using of PHYRE^2 and SWISS-MODEL software

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Abstract. Plants contained a large number of proteins homologous to isoflavone reductase. Two palmae tree genes, c2qx7A and 1qyc1B, encoding isoflavone reductase-like proteins had been previously identified from their unique expression patterns. To gain insight into the possibility of protein modeling of isoflavone reductase, we compared in detail the build models of protein by PHYRE^2 and SWISS-MODEL software. The oil palm showed a higher in sequence identity, sequence similarity, coverage, and Qmean compared to date palm. Homology modelling showed that 294 residue (97% of the amino acid sequence) had been modelling with 100.0% confidence by the single highest scoring template for both oil palm and date palm using PHYRE^2. This coverage was higher than the SWISS-MODEL predicted (80% and 77%). The c2qx7A image patterns were not similar to 1qyc1B, suggesting that different protein functions in the response for each plant.

1. Introduction
Isoflavone reductase is family from proteins that appear a role in plant secondary metabolism based on different NADP, which have the oxidoreductases [1]. One a set to essence biosynthetic isoflavone reductase (IFR) genes that established flavonol synthase to flavonol synthesis, wherein F3′5′H (flavonoid 3′,5′-hydroxylase) to the production within 3′,5′-hydroxylated the flavonoid by phenylalanine synthesis under conditions the tree stress [2]. Isoflavone reductase-like (IRL) proteins also were involved as homeostasis of the reactive oxygen species (OsIRL) expression or overexpression when delivers increase tolerance for plants [3]. This protein was imperative to daidzen biosynthesis also the conversion in NADPH stero-specific 3R reduction suspended isoflavone in stressed plant roots [4].

On the other hand, the protein can be conferring tolerance to oxidative stress in roots [5]. The genes encoding isoflavone reductase protein has contributed to oil palm 33.7 kD as a response of the defense with pathogen Ganoderma boninense [6]. Furthermore, the isoflavone reductase has been reported of 308 amino acids in date palm as allergen protein, and the allergenic potency using for immunotherapy
vaccines materials to human disease [7]. Isoflavone reductase was essential in plant stress response involving in phenylpropanoid synthase, although the phytoalexins synthesis when increasing to tolerance to different abiotic or biotic stresses in plants [8-10]. Accordingly, this study aims to analyze the structure of a protein from isoflavone reductase in oil palm and date palm.

2. Materials and Method

2.1. Protein materials
Isoflavone reductase genes from National Center for Biotechnology Information (NCBI) database protein (https://www.ncbi.nlm.nih.gov/) from Elaeis guineensis (oil palm) and Phoenix dactylifera (date palm) were collected. The Accession numbers sequence of the nucleotide (amino acid) source followed GenBank accession number: XM029268527; XM029268529 (oil palm), and XM008779277; NW008247847 (date palm).

2.2. Protein template sources and build model
The template sources and build a model of the 3-dimensional structure protein was carried out using the PHYRE software (http://www.sbg.bio.ic.ac.uk/~phyre2/html/page.cgi?id=index) [11], and the SWISS-MODEL software (https://swissmodel.expasy.org/) [12]. The highest quality of template has been selected for the builds model.

2.3. Trans-membrane helix prediction
Trans-membrane helices have been predicted in the sequence to adopt the topology using PHYRE software (http://www.sbg.bio.ic.ac.uk/~phyre2/html/page.cgi?id=index), furthermore the cytoplasmic and extracellular sides for membrane was labeled from publication [11]. From the START until the END process of each Trans-membrane helix established of the number indicated to residue index.

3. Results and Discussion

3.1. The protein PHYRE and SWISS-MODEL
The isoflavone reductase protein modeling using PHYRE for oil palm and date palm showed in Table 1. The oil palm and date palm genes have a different result in sequence aligned. The protein ID: c2qx7A of oil palm has a sequence aligned was shown 98.00, whereas the date palm showed 97.00. On the other hand, the results of residue, confidence and coverage had a similar value.

| Gene       | Target ID | Seq. Aligned | Residue | Confidence | Coverage |
|------------|-----------|--------------|---------|------------|----------|
| Oil palm   | c2qx7A    | 98.00        | 294     | 100.00     | 0.97     |
| Date palm  | c2qx7A    | 97.00        | 294     | 100.00     | 0.97     |

Similarly, SWISS-MODEL protein results in the range of protein sequence have obtained the same value for oil palm and date palm derived from 84-308 amino acid (Table 2). The oil palm showed a higher in sequence identity (65.00), the similarity of sequence (0.48), coverage (0.80), and Q-mean (0.41) compared to date palm.

| Gene       | Target ID | Seq. Identity | Seq. Similarity | Range | Coverage | Q-mean |
|------------|-----------|---------------|-----------------|-------|----------|--------|
| Oil palm   | 1qyc1B    | 65.00         | 0.48            | 84-308| 0.80     | 0.41   |
| Date palm  | 1qyc1B    | 50.00         | 0.44            | 84-308| 0.77     | 0.33   |
Other than in the palm trees, the isoflavone accumulation has been reported for the selection of soybean seeds with Quantitative Trait Loci (QTL). Twenty four genes of isoflavone have been reported in the range of 4.20–21.20 average percentage for phenotypic variation [13]. Furthermore, the isoflavone reductase-like protein and chalcone isomerase type A has been a role accumulation as an antioxidant activity to combat the toxicity of the metal in Glycine max [14]. Another case, the short-chain reductase contains isoflavone reductase-like (IRL) protein had a trigger of photobiological in hydrogen production for microalgae [15].

3.2. The PHyre\(^2\) and SWISS image of protein models
Homology modelling showed that 294 residues (97% within the amino acid sequence) resulted 100.0% confidence of modelling from the single highest template scoring in oil palm and date palm using PHyre\(^2\) software (Figure 1A and 1B). The coverage was a higher value compared the SWISS-MODEL predicted 80% and 77% respectively (Figure 2A and 2B).

\[\text{Figure 1. The PHyre}^2\text{ protein modelling for oil palm (A) and date palm (B). Image coloured by rainbow N} \rightarrow \text{C terminus. Model dimensions (Å): X: 43.193 Y: 54.669 Z: 56.702 (A); Model dimensions (Å): X: 52.960 Y: 61.872 Z:47.342 (B)}\]

\[\text{Figure 2. The SWISS-MODEL protein for oil palm (A), and date palm (B).}\]

Isoflavone reductase (homology modelling HsABL1) also has been reported in previous study and analyzed using PHyre\(^2\) software (PDB ID: 2FO0) used as templates. That protein function for the chain was regulated to Fusarium graminearum stress, and as regulatory genes of the biosynthesis of metabolites pathways when the pathogen-infected the plants [16].
3.3. The Trans-membrane helices of the PHYRE$^2$ and SWISS models

Figure 3 showed the Trans-membrane helices in both oil palm and date palm. Both genes had one Trans-membrane helix (S1). The different position between oil palm was on S1 (145-160), and date palm S1 (149-164) in the extracellular and cytoplasmic (N-C terminal). The other invention of isoflavone reductase protein, the full length of cDNA for Oryza sativa genes encoding 486 amino acids of isoflavone reductase (MW: 53.86 kD) was constituted CpPCS protein which is the C-terminal region [17].

![Figure 3. The PHYRE$^2$ Trans-membrane helices of oil palm (A) and date palm (B).](image)

4. Conclusions

Protein modelling purposed for studying distinct isoflavone reductase proteins even in one palm tree species. That protein contributes to the biotic and abiotic stress of the plant. The predict protein modelling image for oil palm and date palm has not similar results using PHYRE$^2$ and SWISS-MODEL software. The oil palm showed a higher for sequence similarity, sequence identity, coverage, and Q-mean compared to date palm.

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