ABSTRACT

The *Elaeis guineensis* Jacq. and the *Elaeis oleifera* are the two species of *Elaeis* genus that supplies the vegetable oil and fats significantly in the world market. Palm oil obtained from *E. guineensis* Jacq. Tenera (*Eg*) contains about 54% of saturated fatty acids, dominated by palmitic acid (44%); however, palm oil obtained from *E. oleifera* (*Eo*) contains 28% saturated fatty acids having palmitic acid only 25%, but, high (69%) oleic acid content in it. Oil (mesocarp) of *Eg* contains only 39% oleic acid. In fatty acid biosynthesis pathway of oil palm, β-ketoacyl-[ACP] synthase II (KASII), KASIII, palmitoyl-[ACP] thioesterase (PATE) and Δ9-stearoyl-[ACP] desaturase (SAD) are known to play important roles. The PATE and KASII enzymes determine the level of palmitic acid and stearoyl-ACPs content respectively. The SAD enzyme determines the level of oleic acid; whereas KASIII enzyme is involved in initial fatty acid chain elongation reactions. To date, nobody has reported the structures and structural features of oil palm KASII, KASIII, PATE and SAD proteins. The objective of this research project was to predict three dimensional (3D) structures of oil palm KASII, KASIII, PATE and SAD proteins using molecular modeling tools to elucidate and understand their unique features. The 3D structures were predicted for both proteins using homology modeling and *ab-initio* technique approach of protein structure prediction. Molecular dynamics (MD) simulation was performed for 30ns to refine the predicted structures as a preparatory process for docking. The predicted structure models were evaluated and root mean square deviation (RMSD) and root mean square fluctuation (RMSF) values were calculated. The stable conformations obtained from the MD simulation were dock to their respective substrate/s (*Eg*KASII, *Eo*KASII with palmitoyl-ACP and malonyl-ACP; *Eg*KASIII, *Eo*KASIII with acetyl-CoA and malonyl-ACP; *Eg*PATE, *Eo*PATE with palmitoyl-ACP; *Eg*SAD, *Eo*SAD with stearoyl-ACP) by Autodock 4.0. The *Eg*KASII, *Eo*KASII, *Eg*KASIII, *Eo*KASIII, *Eg*PATE, *Eo*PATE, *Eg*SAD and *Eo*SAD proteins structure were stereochemically optimized to fix clashes and bad angles which placed the residues at 91.0%, 92.9%, 90.4%, 90.1%, 90.5%, 93.2%, 93.0% and

93.3% respectively, in the core region of Ramachandran plot. The *Eg*KASII, *Eo*KASII, *Eg*KASIII, *Eo*KASIII, *Eg*PATE, *Eo*PATE, *Eg*SAD and *Eo*SAD structures predicted by using *ab-initio* technique approach shows 6.0%, 9.0%, 8.8%, 6.1%, 9.0%, 8.8%, 6.8% and 4.0% deviation to its structures predicted by homology modeling, respectively. The structure refinement and validation confirmed that the predicted structures are accurate. We successfully predicted the 3D structures for oil palm KASII, KASIII, PATE and SAD proteins. The active-site residues in KASII, KASIII, PATE and SAD proteins were also identified. This finding can be extended to experimental validation to access the efficacy of the predicted 3D protein structures.