Functional and Structural Characterization of a Germin-Like Protein from *Calotropis procera* Using In Silico Methods

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INTRODUCTION: Germin and germin-like proteins (GLPs) constitute a large family of plant proteins known to be involved in many stress related processes. True germins have been associated with oxalate oxidase activity, whereas GLPs exhibit superoxide dismutase (SOD) or other activities. Therefore, the study of three dimensional structure of germin and GLPs can be a valuable method to understand the major differences between these two groups of proteins. **OBJECTIVE**: The aim of present study was predict some of the properties and functions of a GLP from *Calotropis procera* by modeling and molecular docking studies. **MATERIAL AND METHODS**: To find germin-like orthologs, we used sequences of different GLPs in a local BLAST search (tBLASTn) querying the assembled *C. procera* transcriptome sequences. Germin-like genes were translated using ExPASy translate tool. The homology modeling program GalaxyWEB server was used to generate the models of target protein. The stereochemical quality of the predicted models was evaluated with PROCHECK by Ramachandran plot analysis. Docking study was performed using substrate oxalate (ligand) in order to study region-specificity of modeled *C. procera* GPL towards oxalate. **RESULTS AND DISCUSSION**: Ramachandran plot analysis of models was obtained by PROCHECK server and the best model in terms of stereochemical quality showed a positive overall G-factor value of 0.0. The total clusters of docking conformations showed negative binding energies. A careful inspection of the binding pocket of GLP model indicated that oxalate adapted a position in a cage surrounded by His107, His109, Glu114 and Phe170 in *C. procera* GLP. Distance of oxalate from N atom of aromatic ring of His 105 and His107 was 4.2 and 3.1 respectively. **CONCLUSIONS:** The GLP from *C. procera* exhibited three histidines and one glutamate in the active site. High docking energies of the model revealed a tight binding of substrate oxalate which can lead to expected catabolic metabolism for degradation of oxalate.

Keywords: Germin-like, Docking, Oxalate oxidase.
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