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Structural characterization of cassava linamarase-linamarin enzyme complex: an integrated computational approach

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Abstract

Cassava linamarase is a hydrolyzing enzyme that belongs to a glycoside hydrolase family 1 (GH1). It is responsible for breaking down linamarin to toxic cyanide. The enzyme provides a defensive mechanism for plants against herbivores and has various applications in many fields. Understanding the structure of linamarase at the molecular level is a key to avail its reaction mechanism. In this study, the three-dimensional (3D) structure of linamarase was built for the first time using homology modelling and used to study its interaction with linamarin. Molecular docking calculations established the binding and orientation nature of linamarin, while molecular dynamics (MD) simulation established protein-ligand complexes' stability. Binding-free energy based on MM/PBSA was further used to rescore the docking results. An ensemble structure was found to be relatively stable compared to the modelled structure. This study sheds light on the exploration of linamarase towards understanding its reaction mechanisms.

Keywords: LinamaraseLinamarinmolecular dynamics simulationmolecular dockingCassava