A Computational Approach to Predict the Regulation of Antioxidant Enzyme, Catalase in the Plant Defence Mechanism

Abstract

Plants defense system protects themselves from pathogens in two ways by preformed mechanisms and through infection-induced responses of the immune system. It is always apparent as a restriction of pathogen growth and spread to a little zone around the infected area. During localized cell death, the visible necrotic lesion evokes up and induces the programmed cell death (apoptosis). Systemic acquired resistance (SAR) will be helpful to the infected plants after a period of 5-7 days. Salicylic acid (SA) is a plant hormone essential for the immunity in plants. SA has been found to involve in the control of microbe/pathogen-associated molecular pattern triggered immunity, effector-triggered immunity
and system acquired resistance (SAR). The binding modes and the bonding pattern between salicylic acid and the enzyme catalase is still unknown. In our study, the different binding modes of salicylic acid in different pockets were analyzed. Among the chosen pockets, the best probable binding pocket was identified computationally based on the binding energy, intra-molecular energy, internal energy and inhibition constant between two molecules.

References

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