Revealing the Structural and Dynamic Properties of Betaine Aldehyde Dehydrogenase 2 from Rice (Oryza sativa): Simulation Studies

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Abstract : Betaine aldehyde dehydrogenase 2 (BADH2) is an enzyme that inhibits the accumulation of 2-acetyl-1-pyrroline (2AP), a potent flavor compound in rice fragrance. BADH2 contains three domains (NAD-binding, substrate-binding, and oligomerization domains). It catalyzes the oxidation of amino aldehydes. The lack of BADH2 results in the formation of 2AP and consequently an increase in rice fragrance. To date, inadequate data on BADH2 structure and function are available. An insight into the nature of BADH2 can serve as one of key starting points for the production of high quality fragrant rice. In this study, we therefore constructed the homology model of BADH2 and employed 500-ns Molecular Dynamics simulations (MD) to primarily understand the structural and dynamic properties of BADH2. Initially, Ramachandran plot confirms the good quality of modeled protein structure. Principle Component Analysis (PCA) was also calculated to capture the protein dynamics. Among 3 domains, the results show that NAD binding site is found to be more flexible. Moreover, interactions from key amino acids (N162, E260, C294, and Y419) that are crucial for function are investigated.

Keywords : betaine aldehyde dehydrogenase 2, fragrant rice, homology modeling, molecular dynamics simulations
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