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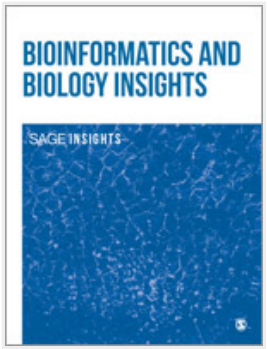

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SAGE Video
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SAGE Knowledge
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The ultimate methods library

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CQ Library
American political resources

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Computational Model of the Effect of a Surface-Binding Site on the *Saccharomycopsis fibuliger*a R64 α-Amylase to the Substrate Adsorption

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ABSTRACT: α-Amylase is one of the important enzymes in the starch-processing industry. However, starch processing requires high temperature, thus resulting in high cost. The high adsorptivity of α-amylase to the substrate allows this enzyme to digest the starch at a lower temperature. α-Amylase from *Saccharomycopsis fibuliger*a R64 (Sfamy R64), a locally sourced enzyme from Indonesia, has a high amylolytic activity but low starch adsorptivity. The objective of this study was to design a computational model of Sfamy R64 with increased starch adsorptivity using bioinformatics method. The model structure of Sfamy R64 was compared with the positive control, ie, *Aspergillus niger* α-amylase. The structural comparison showed that Sfamy R64 lacks the surface-binding site (SBS). An SBS was introduced to the structure of Sfamy R64 by S383Y/S386W mutations. The dynamics and binding affinity of the SBS of mutant to the substrate were also improved and comparable with that of the positive control.

KEYWORDS: α-amylase, starch adsorptivity, molecular dynamics simulation, surface-binding site, *Saccharomycopsis fibuliger*a R64

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Introduction

α-Amylase, or 1,4-α-D-glucan glucanohydrolase, catalyzes the cleavage of α-1,4 glycosidic linkage in starch to yield maltotriose, maltose, glucose, and limit dextrin.[1] This enzyme has many applications in the industrial processes such as food, fermentation, textile, paper, detergent, and pharmaceuticals.[2] It is noted that α-amylase constitutes 25% of the enzyme market.[3] In starch-based industry, α-amylase is used to break down the starch granules, which are densely packed in a polycrystalline state by inter- and intramolecular bonds. Starch granules are insoluble in cold water and often resistant to chemicals and enzymes treatment.[4] Therefore, a gelatinization step at a high temperature (105°C) is needed to open the crystalline structure of starch for easier enzymatic digestion.[5] However, this high-energy process increases the cost of production.[6] Therefore, to avoid or to reduce the gelatinization temperature by direct hydrolysis of raw starch is interesting to be investigated.[5,7,8] Many studies showed that the raw starch–digesting ability of amylase was affected by the presence of carbohydrate-binding module (CBM) or starch-binding domain (SBD) and the binding sites on the protein surface, namely, surface-binding site (SBS).[8,9] The CBM is a separate binding module, whereas SBS is a site on the catalytic module itself. These structural features are essentials to the substrate adsorption of the amylase.[9]

The raw starch–digesting amylases are mostly produced by fungi, such as *Aspergillus* sp., *Rhizopus* sp., and *Corticium rolfsii*.[7,8] In Indonesia, the best identified amylolytic enzyme–producing microorganism was a strain of *Saccharomycopsis fibuliger*a R64.[10] However, at the enzymatic level, the isolated α-amylase from *S fibuliger*a R64 (Sfamy R64) showed no adsorption to the raw starch.[11] Thus, unlike the other raw starch–digesting α-amylase, Sfamy R64, is predicted without the SBD and/or SBS. Unfortunately, the structure of Sfamy R64 is still not available.

Computer-Aided Molecular Design (CAMD) is one of the promising methods to develop a modified enzyme with desired properties. Fungamyl, a thermostable amylase-like enzyme at acidic pH, is one of the successful products which was engineered using CAMD technique.[12] Therefore, to improve the substrate adsorption of Sfamy R64 without compromising its excellent amylolytic activity is expected to be achieved by CAMD approach. In this study, we used the crystal structure of *Aspergillus niger* α-amylase, which shares 71% homology with Sfamy R64, as a positive control. It has one SBS in the C-domain which is bound to maltose. The complex structure was resolved at 1.8 Å resolution.[13]

Therefore, this study aims to investigate the effect of new SBS on the model structure of Sfamy R64 toward the substrate adsorption using computational methods. The model was developed using homology modeling method. The structural dynamics behavior of Sfamy R64 as compared with the positive