MOLECULAR DOCKING AND KINETIC STUDY OF TRANSGLYCOSYLATION REACTION FOR NARINGENIN USING AMYLOSUCRASE FROM DEINOCOCCUS WULUMUQIENSIS

Dong-Ho Seo, Graduate School of Biotechnology and Institute of Life Science and Resources, Kyung Hee University, Republic of Korea
dhseo@khu.ac.kr
Su-Jeong Yu, Department of Food Science and Technology, College of Agriculture and Life Sciences, Jeonbuk National University, Republic of Korea
Cheon-Seok Park, Graduate School of Biotechnology and Institute of Life Science and Resources, Kyung Hee University, Republic of Korea

Amylosucrase (ASase, E.C. 2.4.1.4) efficiently biosynthesizes α-glucoside by using various flavonoids as acceptor molecules and sucrose as a donor molecule, instead of expensive substrates like UDP- and ATP-glucose. Flavonoid α-glucosides have higher water solubility and stability compared to aglycone form. In this study, ASase from *Deinococcus wulumuqiensis* (DwAS) biosynthesized more naringenin α-glucoside (NαG) with sucrose and naringenin as donor and acceptor molecules, respectively, compared to other ASase from *Deinococcus* sp. Docking simulations showed that the DwAS had a more accessible active site for naringenin compared to ASase from *Deinococcus geothermalis* (DgAS). The 217th valine in DwAS was an isoleucine at the 221st valine in DgAS, and the isoleucine was predicted to prevent naringenin from accessing the active site. The DwAS V271I variant had a significantly reduced biosynthetic rate of NαG compared to the wild-type. The DwAS exhibited a decrease in the fluidity of loop 7, which is involved in the formation of the active site topology and contains subsite +1 residues, compared to DgAS through molecular dynamics analysis. In the presence of naringenin, k_{cat}/K_m of DwAS and DgAS was determined to be 3.759 $min^{-1}\cdot mM^{-1}$ and 1.085 $min^{-1}\cdot mM^{-1}$, respectively. In the presence of sucrose, k_{cat}/K_m of DwAS and DgAS was determined to be 0.536 $min^{-1}\cdot mM^{-1}$ and 0.264 $min^{-1}\cdot mM^{-1}$, respectively. These results showed that DwAS has a higher transglycosylation activity for naringenin than DgAS.