Poster Presentation

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Structural insights into the production of 3-HP by AbKGSADH

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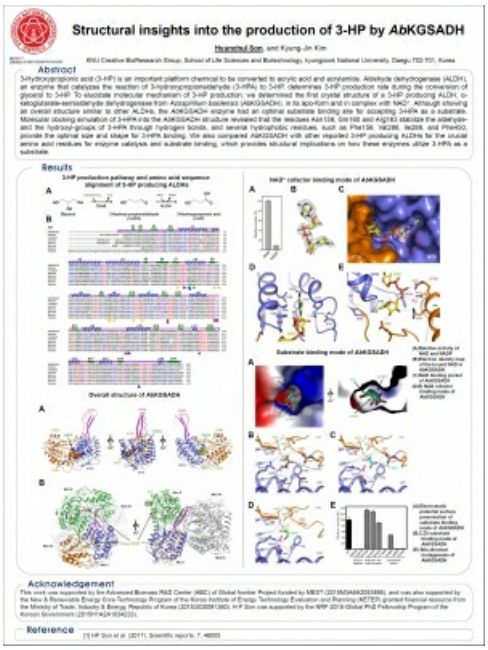
3-Hydroxypropionic acid (3-HP) is an important platform chemical to be converted to acrylic acid and acrylamide. Aldehyde dehydrogenase (ALDH), an enzyme that catalyzes the reaction of 3-hydroxypropionaldehyde (3-HPA) to 3-HP, determines 3-HP production rate during the conversion of glycerol to 3-HP. To elucidate molecular mechanism of 3-HP production, we determined the first crystal structure of a 3-HP producing ALDH, α-ketoglutarate-semialdehyde dehydrogenase from Azospirillum basilensis (AbKGSADH), in its apo-form and in complex with NAD+. Although showing an overall structure similar to other ALDHs, the AbKGSADH enzyme had an optimal substrate binding site for accepting 3-HPA as a substrate. Molecular docking simulation of 3-HPA into the AbKGSADH structure revealed that the residues Asn159, Gln160 and Arg163 stabilize the aldehyde- and the hydroxyl-groups of 3-HPA through hydrogen bonds, and several hydrophobic residues, such as Phe156, Val286, Ile288, and Phe450, provide the optimal size and shape for 3-HPA binding. We also compared AbKGSADH with other reported 3-HP producing ALDHs for the crucial amino acid residues for enzyme catalysis and substrate binding, which provides structural implications on how these enzymes utilize 3-HPA as a substrate.
[1] HF Son et al. (2017). Scientific reports, 7, 46005



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