

The relationship between substituted alkyl chain length of imidazolium-based ionic liquids and structural change of CALB: a combined in silico and in vitro study

엄도영, 김호신<sup>1</sup>, 구윤모\*

인하대학교; <sup>1</sup>North Carolina State University

(ymkoo@inha.ac.kr\*)

Ionic liquids(ILs) are used as the solvents for the study. We find that alkyl chain length of cation with imidazolium affects structural change and enzymatic reaction of Candida Antarctica Lipase B (CALB). In order to obtain accurate reliability on enzyme activity, we performs molecular dynamic simulation carrying out experimental methods. Our experimental data shows initial reaction and conversion rate in the following order: [BMIM][TfO] > [HMIM][TfO] > [OMIM][TfO] > [EMIM][TfO]. We calculates the distance from the center of mass between ILE-189 and ILE-285, which can play a role as an entrance of catalytic cavity. The probability distribution of the length among these two amino acids is located around the distance at initial structure, which is 11.36Å, except in the case of [EMIM][TfO]. In addition, the conformational changes of the active site are observed in the case of [OMIM][MS]. Moreover, we investigates that amino acid structures of ILE-285, VAL-286, ALA-287 around the active site maintain helix structure, but [EMIM][TfO] changes helix to turn structure.