Analysis of the Conformational Changes of *Candida antarctica* Lipase B in Ionic Liquids

김호신, Latsavongsakda Sethaphong[1], 하성호[2],
Yaroslava G. Yingling[1], 구윤모*
인하대학교; [1]North Carolina State Univ.; [2]한남대학교
(ymkoo@inha.ac.kr*)

In order to investigate the mechanisms of interaction between ILs and CALB, as well as to compare structural changes of CALB in ILs with that in organic solvent, molecular dynamics simulation study was performed. The results represented that the type of solvent molecule plays a pivotal role in conformational changes of active site of CLAB and its cavity region. Especially ILE-189 and ILE-285 located in entrance of cavity was affected by interaction with solvent, and acted as a gate molecule which impedes or permit the incoming and outgoing of substrates into cavity. These two amino acids maintained their structural position in [Bmim][TfO] compared with initial one measured by X-ray diffraction. On the other hand, two amino acids were getting close as time passes, and then make close conformation in [Bmim][Cl]. In case of *tert*-butanol, although the gate has been in open state during the simulation, structure of amino acids reside in inner part of active site funnel has been changed, thus yielding to decrease in enzyme activity. To support the results of simulation study, trans-esterification reaction was carried out by using CALB in ILs and *tert*-butanol.