Molecular Modeling and Simulation for Lipase-catalyzed Esterification of Structural Isomeric Butanols

정정영, 권정훈, 강정원*
고려대학교
(jwkang@korea.ac.kr*)

The lipase-catalyzed esterification reactions of structural isomeric butanols (normal-, iso-, sec-, tert-) and butyric acid were investigated by quantum mechanical and molecular dynamics simulation analysis. The whole reaction pathways and reaction rates were predicted on the model system of *Candida Antarctica* lipase B (CALB) with substrates using the energy profiles through quantum mechanical calculation. Conformational preference of enantiomers was analyzed using the molecular dynamics simulation analysis. Calculated results from molecular modeling studies have been compared qualitatively with experimental data using CALB and substrates.