분자역학 방법을 이용한 lipase 효소의 비수용성 용매 상에서의 반응 메커니즘의 모델링

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Lipases are widely used in organic synthesis, chiral synthesis, modification of fats and oils, etc. The enzyme reaction mechanism is an important factor in design and operating such processes. Due to difficulties of finding the transition state of reaction and calculating energy of an intermediate, it is difficult to explain the whole reaction mechanism using experimental study. Molecular modeling using computer can be used as an alternative method.
CHARMM Force field (http://www.charmm.org/) known as a suitable macromolecular calculation was applied to the enzyme system. The reaction mechanism was investigated using conformational changes and accompanying energy barriers. The reactant-enzyme intermediate structure of Candida antarctica Lipase B (Novozyme 435) and acetates was studied using molecular dynamics simulation. The information about reaction mechanism was discussed from the analysis of the trajectories.