The effect of initial water activity of MTBE (methyl tert-butyl ether) medium on CALB (Candida antarctica lipase B) catalyzed esterification reaction is investigated using experimental methods and classical molecular dynamics (MD) simulations. The experimental kinetic studies show that the initial reaction rate of CALB-catalyzed esterification reaction between butyric acid and ethanol decreases with increasing initial water activity of the medium. The highest rate of esterification is observed at the lowest water activity studied. MD simulations were performed to gain a molecular insight on the effect of initial water activity on the rate of CALB-catalyzed reaction. Our results show that hydration has an insignificant effect on the structure and flexibility of CALB. Rather, it appears that water molecules bind to certain regions ("hot spots") on the CALB surface and form clusters. The size of the water clusters at these hot spot regions gradually increase and expand with increasing water activity. Consequently, the surface area of CALB covered by the water molecules also increases. Specifically, our results indicate that a particular water cluster located close to the active site partially cover the binding pocket of substrate at high water activity. As a consequence, the effective concentration of substrate at the catalytic site decreases. Therefore, the reaction rate slows down with increasing water activity, which correlates well with the observed decrease in the experimentally determined initial reaction rate.

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