

The open lid conformation of the lipase is explored in the compressed gas: New insights from molecular dynamic simulation

The Journal of Molecular Catalysis B: Enzymatic

The advantages of enzymatic reactions in compressed gases such as supercritical CO₂ are limited due to the enzyme inactivation. But recent experimental observations reported the high activity of enzymes such as lipases in compressed propane. But there are no clear reasons at the molecular levels for such behavior. In this work using molecular dynamic simulation, we showed for the first time the possibility of interfacial activation of lipases in a compressed gas. The analysis showed that in compressed propane the lid of the lipase was opened and so the active conformation of the enzyme was resulted. Moreover it is found that in the compressed propane, similar to the aqueous solution, the enzyme has native conformation.

Enzyme is stabilized by a protection layer of ionic liquids in supercritical CO₂: Insights from molecular dynamic simulation