Ultrasonic enhancement of lipase-catalyzed reactions: Mechanistic investigation using molecular docking analysis

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Abstract

Ultrasound has emerged as an efficient green technology for intensification of lipase-catalyzed processes. These processes are of high significance in the context of renewable fuels synthesis. In this paper, we have attempted to reveal the molecular mechanism of sonication-induced enhancement of lipase-catalysed reactions. Using hybrid quantum mechanics/ molecular mechanics computations, we have initially determined the structure and amino acid composition of the binding pockets of two common lipase enzyme, viz. *CALB* and *TLL*. Next, these binding pockets were visualized using softwares PyMOL and VMD to deduce their location in different motifs of the secondary structure of lipases. Finally, the docking analysis of different ligands was performed to reveal the amino acid residues involved for each ligand and the nature of their interactions. Our results revealed that most of the binding pockets are located in the α-helix and random coil motifs of enzyme and binding interactions are of the type hydrogen bond and hydrophobic interactions. Previous literature reports significant rise in α-helix and random coil contents of lipases with sonication. This observation concurs with our analysis, and suggests rise in enzyme activity with sonication due to widening of catalytic cavity and easier accessibility to binding pockets. Thus, our analysis provides molecular-level insight into the sonication-induced enhancement in kinetics and yield of lipase-catalyzed reactions.

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