

Mechanistic investigations in sonoenzymatic synthesis of n-butyl levulinate

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Abstract

n-Butyl levulinate (n-BL) has numerous applications in biofuel and green solvents. In this paper, we have reported mechanistic accounts of sonoenzymatic synthesis of n-BL using Novozym 435. Esterification parameters were optimized with statistical design of experiments. Application of 35 kHz sonication boosted n-BL yield from 70.9% to 92.22%. Mechanistic investigation using Ping-Pong Bi-Bi kinetics model and molecular docking simulations revealed interesting influence of sonication on esterification reaction. Exposure to sonication induced significant changes in the secondary structure of enzyme, as revealed in ATR-FTIR analysis. Sonication increased α -helix content of enzyme that increased enzyme activity by opening of flapping lid and widening the catalytic cavity. Sonication also caused unfolding of secondary structural motifs with rise in random coil content that favored formation of enzyme-ligand complexes. These effects enhanced reaction velocity and substrate affinity with reduction in inhibition and unfavorable dissociation of intermediate complexes, which ultimately enhanced n-BL yield.

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