Electronic Journal of Biotechnology
E-ISSN: 0717-3458
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Pontificia Universidad Católica de Valparaíso
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Lipase-catalyzed enantioselective esterification of flurbiprofen with n-butanol
Electronic Journal of Biotechnology, vol. 3, núm. 3, diciembre, 2000, pp. 195-201
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Abstract

The influences of water activity and solvent hydrophobicity on the kinetics of the lipase-catalyzed enantioselective esterification of flurbiprofen with n-butanol were investigated. The solvent effect was not similar for lipases from Candida rugosa (Crl), Mucor javanicus (Mjl), and porcine pancreas (Ppl). The lipase-catalyzed reaction rates in different solvents across a wide range of water activities revealed that the Ppl-catalyzed reaction exhibited no enantioselectivity and no substantial water activity or solvent dependence. The Mjl-catalyzed reaction proceeded faster, preferring the R-enantiomer reaction over that of its antipode, but had little solvent or water activity dependence. The Crl-catalyzed reactions in n-heptane and n-nonane had similar water activity dependence, but the reaction was considerably faster and more enantioselective (preferring the S-enantiomer reaction) in isooctane, a solvent whose hydrophobicity is intermediate between that of the other two alkanes. Substrate enantiomeric excess, for the Crl-catalyzed reaction at 96 hours and at a water activity of 0.65, in n-heptane, isooctane, and n-nonane was 40.9, 93.0, and 50.0%, respectively. Since the three solvents possess similar physical properties, the explanation for this anomalous behavior might be the effect of the solvent structural characteristics on Crl, since isooctane is the only branched alkane.

Keywords

Enantioselectivity, esterification, flurbiprofen, lipase, solvent dependence, water activity.