

Influence of ionic liquid properties on enzyme activity and enantioselectivity

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Abstract

Room-temperature ionic liquids (ILs) are attracting growing interest as alternative reaction media for catalytic transformations, which are non-volatile, highly polar and thermally stable. Here, we discuss their use as reaction media for biocatalysis. The initial rate and enantioselectivity of lipase-catalyzed esterification of profens in ILs were measured and compared with those obtained in conventional organic solvents. ILs used in this study include 1-alkyl-3-methylimidazolium with a variety of anions including $[\text{Tf}_2\text{N}]^-$, $[\text{SbF}_6]^-$, $[\text{PF}_6]^-$, $[\text{BF}_4]^-$ and $[\text{TfO}]^-$. In addition, Kamlet-Taft solvatochromatic parameters, $\log P$, refractive indices and Hildebrand solubility parameters for ILs have been determined. And then, a multiparameter correlation method for predicting the effects of ILs on enzyme activity and enantioselectivity is presented. The polarity/polarizability of the ILs studied is similar to that of dimethylsulfoxide (DMSO) and dimethylformamide (DMF) and is slightly higher than that of short chain alcohols. The acidity of the ILs is less than that of most short chain alcohols, whereas the basicity of the ILs studied here varies widely. The $\log P$ values for ILs tested ranged between -2.39 and 1.42. Both cations and anions of ILs considerably affect the $\log P$ values. The effect of anion was dominant in determining the initial reaction rate of enzymatic kinetic resolution in ILs. No enzymatic activity was shown in DMSO and DMF which have similar polarity to ILs. Several ILs, which indicates that ILs can be used as an alternative to conventional organic solvents showed comparable or higher initial rates. Initial reaction rate and enantioselectivity of lipase Novozym 435 could be correlated with a linear solvation relationship equation using five parameters (dispersion, polarity, acidity, basicity and molar cohesion energy density).

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