

Influence of ionic liquid properties on enzyme activity and enantioselectivity

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Room-temperature ionic liquids (ILs), which are non-volatile, thermally stable and highly polar, are attracting growing interest as alternatives to conventional organic solvents. Here, we discuss their use as reaction media for biocatalysis. The initial rate and enantioselectivity of lipase-catalyzed esterification of 2-arylpropionic acids 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 $[\text{BF}_4]^-$, $[\text{PF}_6]^-$, $[\text{SbF}_6]^-$, $[\text{Tf}_2\text{N}]^-$ and $[\text{TfO}]^-$. In addition, Kamlet-Taft solvatochromatic parameters, refractive indices, Hildebrand solubility parameters and $\log P$ 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 effect of anion was dominant in determining the initial reaction rate of enzymatic kinetic resolution in ILs. Initial reaction rate and enantioselectivity of lipase could be correlated with a linear solvation energy relationship equation using five parameters (dispersion, polarity, acidity, basicity and molar cohesion energy density).