Lipase-catalyzed synthesis of benzyl hexanoate by using ionic liquid as reaction media in controlled water activity system

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Abstract

Room-temperature ionic liquids (ILs) are attracting growing interest as reaction media for catalytic transformations, which non-volatile, highly polar and thermally stable. Here, we discuss their use as reaction media for biocatalysis. When enzymatic reaction is performed in nonaqueous media, water plays an important role in enzyme dynamics. Water also participates in the reactions which lead to denaturation. Therefore, water content of the ILs must be considered when investigating the enzymatic reaction in nonaqueous media. Direct esterification of carboxylic acids and alcohols using lipase is an industrially useful system. However, removal of water is generally needed for satisfactory conversion. In this work, the effect of water activity on the lipase (Lipozyme IM)-catalyzed synthesis of benzyl hexanoate (food additive) in [C₄mim][PF₆] was investigated by using computer-aided water activity control system. There was an optimal water activity for initial reaction rates at 0.6. Meanwhile, the final equilibrium conversion reaches maximum at low initial water activity (under 0.1), which is about two times higher than that obtained at high initial water activity (over 0.9). Therefore, water content of the reaction mixture was monitored and controlled to obtain high reaction rate and high yield. Under the optimal conditions with water activity control, the synthetic yield of ester was enhanced from 50% to 81%.

References

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