426j Solvent Strategies of Asymmetric Reducing Synthesis Ethyl (R) -2-Hydroxy-4-Phenylbutyrate Catalyzed by Yeast

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The asymmetric reducation of ethyl-2-oxo-4-phenylbutyrate (OPBE) catalyzed by Saccharomyces cerevisiae in organic solvent, water/organic diphase system and water/ionic liquid system to synthesize optical active ethyl-2-hydroxy-4-phenylbutyrate (HPBE) was investigated, respectively.

The reaction was executed in aqueous diethyl ether at pH7.0, 30 ^{o}C for 24h under catalysis of the yeast which was pre-incubated for 2h in the presence of phenacyl chloride, reached a yield of 75.82% and a stereo-selectivity of 82.25% (e.e.). The amount of water in the media and the substrate(OPBE) concentration was 30 g/L and 5 mmol/L, respectively.

The effect of different solvents on enantioselectivity was examined. The effects of the hydrophobicity of organic solvent, volume ratio of water phase to organic phase, reaction time, temperature, pH and ionic strength, sucrose concentration, etc. on conversion of OPBE, yield of HPBE and ee of the product were systematically investigated. Benzene is found to be the best organic solvent for the reaction. The optimum reaction conditions, such as, volume ratio of water phase to organic phase, reaction time, reaction temperature, pH and sucrose concentration are: 1/2, 15h, 28~32 ^{o}C, 8 and 100g/L respectively, the stereoselectivity for the asymmetric reduction was increased further with the use of phenacyl chloride, under which the conversion of OPBE, yield of HPBE and ee of the product are as high as 95.06%, 70.62% and 95.06% respectively.

The protential of blending ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate) with water for an efficient and clean processing process was studied. It was shown that the product asymmetrically catalysed by the yeast was (S)-HPBE(-27.66% e.e.) in ionic liquid at very low water concentrations(2% (v/v)), but the selectivity of the yeast was totally changed in water/ionic liquid biphase systems(6.64% e.e.).

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