

INVESTIGATION of RESPONSE SURFACE OPTIMIZATION of BENZOIN SYNTHESIS in SUPERCRITICAL CARBONDIOXIDE

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Abstract

Chiral α -hydroxy ketones are important structural units in many biologically active compounds and they are versatile building blocks in asymmetric synthesis [1]. The biological effect of chiral compounds is dependent one of the enantiomers, so it is important to produce in enantiomerically pure form. Enzymes are used as chiral catalysis because of their high selectivity. The resolution of enantiomers by enantioselective synthesis with enzymes has been exploited extensively for twenty years. Especially interest in the use of lipases as synthetic chiral catalyst has risen rapidly. Because of their ability to catalyze reactions, in organic as well as in aqueous systems, lipases lead to the enantioselective synthesis of wide variety of compounds via hydrolysis, esterification and transesterification [2]. The enzymes employed in most of the work involving supercritical fluids, and more specifically, carbon dioxide, are also lipases [3].

In this work, the enzymatic hydrolysis of chiral benzoin, one of the important α -hydroxy ketones, from racemic benzoyl benzoin to obtain with high enantiomeric excess (ee) was investigated. It is the first study to synthesize benzoin in supercritical carbon dioxide (SCCO₂). Optimization of enantiomeric excess value of benzoin in the enzymatic hydrolysis of benzoyl-benzoin catalyzed by *Candida cylindracea* (CCL) lipase has been carried out in SCCO₂ using response surface methodology (RSM). It was found that CCL lipase enantioselectively hydrolyzed the (R)-benzoin in supercritical media, while it was not catalyzed the reaction at atmospheric conditions. The parameters were temperature (35 - 45 °C), pressure (70-90 bar) and pH (5-9) of the reaction media. Macanova software (version 4.07, Minnesota, USA) was used for regression and graphical analyses of the data obtained. Optimum conditions was found as 40 °C, 79 bar, 6,4 pH and at these conditions enantiomeric excess was obtained as 62 %. Experiments duplicated and same results were achieved, therefore accuracy of the model was tested.

Keywords: Supercritical CO₂, chiral compounds, benzoin, enzymatic reactions

References

- [1]. A. S. Demir, O. Sesenoğlu, *Organic Letters*, 4 12 (2002), 2021-2023.
- [2]. N. Mase, T. Sako, Y. Horikawa and K. Takabe, *Tetrahedron Letters* 44 (2003) 5175-5178.
- [3]. A. J. Mesiano, E. J. Beckman and A. J. Russell, *Chem. Rev.* 99 (1999) 623-633.

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