Influence of solvent suitability in lipase-catalyzed esterification reactions

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Abstract

Esterification reaction in microaqueous system was evaluated using an organic solvents. Lipase-catalyzed esterification reaction was occupied semicontinuously reaction in packed bed reactor. Lipase enzyme used in this research was Novozyme® 435. Solvent system was developed in order to overcome the solubility limitation of both the reagents, glycerol and fatty acid, and to obtain a homogeneous system capable of working in semicontinuous way. Solvents used in this research had log P (partitioning coefficient of solvent between 1-octanol and water) values 3.5 and 0.4. The aim of this research was to know influence of solvent log P values on yield monoglycerides product and content. Based on the research known that mixture solvent log P values used for reaction between glycerol and lauric acid was 1.33. The yield and content of Monoglycerides products was 81.09% and 83.15%, respectively. Although solvent log P values tend to polar, but still had very good activity in lipase-catalyzed esterification reactions in microaqueous system. It promotes the water withdrawal from the medium, preventing a possible deactivation of the enzyme and increasing the conversion of substrates into desired products.

Keywords: Lipase; esterification reaction; organic solvents; solvent suitability

Introduction

Solvents offered the possibility of a reverse reaction of hydrolysis, esterification using free fatty acids (FFA), or transesterification using esters. For that purpose conditions are needed, in which the enzyme will catalyze the synthesis reaction rather than the hydrolysis. Most important, low water content and low water activity are necessary to achieve a high-yield formation of monoglyceride (MG) and the suppression of undesired hydrolysis. Janssen et al. (1993) found that a higher monoester formation was possible with short-chain fatty acid in polar solvent, whereas a higher di- and triester synthesis took place with longer-chain fatty acids in nonpolar organic solvents. The ester molar fractions at equilibrium were found to depend on the fatty chain length in the absence of a solvent.

Monoglyceride was nonionic emulsifiers widely used in the food and pharmaceutical industries. They are also of great interest in synthetic organic chemistry where they are utilized as synthetic intermediates and as chiral building blocks (Berger & Schneide 1992). The monoglyceride obtained in this work, also presents biological activity. It is effective against several lipid-coated viruses, a class which includes the AIDS virus, and against certain bacteria. Monoglycerides can be synthesized at 200–250°C using several metallic catalysts but this leads to a number of unwanted side products and the reaction occurs in a random manner with the formation of mono-, di-, and triacylglycerol.

The formation of isomers of sn-1-monoglyceride and of sn-1,3-diacylglycerol, sn-2-monoglyceride and sn-1,2-diacylglycerol, respectively, can also occur, as shown in Figure 1.

Lipases show a good stability and activity in hydrophobic solvents with 2 < log P < 4, like n-hexane (Laane et al. 1987), but in this medium, glycerol is insoluble. Hydrophobicity parameters were used log P values of solvents. Log P is partitioning coefficient of solvent between 1-octanol and water. The enzymatic esterification of glycerol in polar solvents or its mixture with n-hexane have been used. For example, Janssen et al. (1993) have observed that the use of tertiary alcohols with log P < 2 favors the synthesis of monoesters. The use of n-hexane supplemented with 2-methyl-2-butanol (Bellot et al., 2001) and with glycerol adsorbed on dried silica gel (Castillo et al. 1998) increased the specific production of monoester.

A suitable solvent system to improve miscibility of substrates will result in a more homogenous system and enhance the conversion of substrates, the reaction rate, and the product distribution in favor monoglyceric formation (Kaewthong dan Kittikun, 2004). Solvents such as n-hexane, n-heptane, dioxane, acetonitrile, acetone, isooctane, 2-methyl-2-propanol (tert-butanol), 2-methyl-2butanol (tert-pentanol), or mixtures of some of them are useful in different lipase-catalyzed inesterification reactions (Damstrup et al., 2005).