CURRENT RESEARCH AND DEVELOPMENT IN BIOTECHNOLOGY ENGINEERING AT IIUM

VOLUME II

Editors:

Ibrahim Ali Noorbatcha
Hamzah Mohd. Salleh
Mohamed Elwathig Saeed Mirghani
Raha Ahmad Raus

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CHAPTER 11

MOLECULAR MODELING OF THE BIODEGRADATION POLYESTERS USING LIPASE

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ABSTRACT

The main chain polymers such as polyesters can be biodegraded by various microorganisms. Lipases are among the enzymes that can catalyze hydrolysis of lipid esters (triacylglycerol hydrolases). *Candida rugosa* lipase is commonly used n several biotechnological applications, because the source organism, *Candida rugosa* is well known and considered non-pathogenic and non toxigenic. We have modeled the active site and transition state of the *Candida rugosa* lipase for the degradation of polyesters. These results suggest that mutation at Glu450 will increase the binding strength at the active site lading to increase the activity of the lipase.

Keywords: Lipase, Molecular modeling, *Candida rugosa*, lipid esters, active site

INTRODUCTION

Synthetic polyesters are being continuously used to substitute natural polyesters in almost every area due to its stability and durability. The dramatically increased production of polyesters in combination with their durability leads to increasing littering and world's waste management problems. Aromatic polyesters such as polyethyelene terephthalate (PET) or polybutylene terephthalate (PBT) in contrast were still considered as inert against any biological attack. Recently, Muller (2006) found that *Thermobifida fusca* hydrolase was capable to degrade commercial PET from beverage bottles. Since the complex structure of the enzyme was not available, the active site of the enzyme was assumed as typical as serine hydrolases. Another enzyme that can degrade polyethylene terephthalate (PET) is cutinase from *F. solani pisi*.

Candida rugosa lipase shows an enormous potential for biotechnological applications. As evidenced by the current literature, *Candida rugosa* lipase claims more applications than any other biocatalyst. Its role in the food and flavour industry, the production of ice cream and single cell protein, biocatalytic resolution of life-saving pharmaceuticals, carbohydrate esters and amino acid derivatives unobtainable by conventional chemical synthesis, potent biocide making, biosensor modulations, eco-friendly approach and bioremediation, biosurfactants in detergent