Structural properties of a novel Bacillus carboxylesterase

Esterhuyse JL*, Nthangeni M.B and Litthauer D.

Department of Microbial, Biochemical and Food Biotechnology, University of the Free State, P. O. BOX 339, BLOEMFONTEIN, 9300, SOUTH AFRICA

Carboxylesterases (EC 3.1.1.1) catalyze various industrially important reactions that involve stereoselective synthesis or cleavage of ester bonds. We have cloned from the genomic DNA of Bacillus licheniformis a 3000 bp DNA fragment consisting of an open reading frame of 484 amino acids that showed lipolytic activity on tributyrin-agar growth medium. The protein sequence showed maximum amino acid identity of about 60

3 D structure modelling with p-nitrobenzyl esterase from Bacillus subtilis as template was performed using WhatIf. The model was optimised using a steepest decent minimisation followed by simulated annealing. The loops at the entrance of the binding cavity are variable with a two amino acid deletion leading to one of the loops being shorter, compared to the template. In spite of only 54