

Structure-function relationships of novel and chimeric Family VII bacterial carboxylesterases

Nthangeni, M.B., Tlou, M.G., van Heerden, E., Esterhyse, J 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.) catalyse various industrially important reactions that involve stereoselective synthesis or cleavage of ester bonds. We have cloned from the genomic DNA of *Bacillus* species carboxylesterase (CEST) genes that belong to Family VII of bacterial lipolytic enzymes. The genes contained ORFs of 484-489 amino acid residues and the characteristic GESAG esterase motif. The CEST from *Bacillus pumilus* was 98

3 D structure modeling with p-nitrobenzyl esterase from *Bacillus subtilis* as template was performed using WhatIf and optimisation of the structure using YASARA. An analysis of the binding pockets and the different domains of the native and chimeric enzymes were made and the different kinetic properties are reported relative to their three-dimensional structures.