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BOOK OF ABSTRACTS

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In Silico Determination of Sn-2 Specific Lipase Activity: Alternative Strategy of Lipid Modification

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Lipases (EC 3.1.1.3) are the third most commercialised enzymes, converting oil into free fatty acids and glycerol. Sn-2 stereospecific lipases have lately gained attention due to their particular lipid modifying properties. Triacylglycerol digestion by Sn-2 stereospecific lipase leads to produce one 1,3-diacylglycerol and one free fatty acid. In silico approach is the first step to identify different genes coding for lipase in a particular organism. Gene hierarchy organisation indicates ancient gene duplication and divergence, making theoretical and analytical methods from phylogenetic systems applicable to comparative genomic studies. In this present study, firstly it was observed that the structure obtained via Pymol is 91% confidently modelled (420 residues out of 460; approximately). From CDD BLAST it was found that this protein belongs to alpha/beta hydrolase family with an abhydrolase super family domain. Then a multiple sequence alignment program was run to find the sequence similarity. After that, by using Swissmodel, Alpha fold and Phyre 2.0 the several homology modellings were done. Next, Model validation results were obtained from QMEAN4. PROCHECK, ROQ, ProSA and ERRAT servers. And finally, to check the lipolytic activity of the concerned protein a docking was performed using Autodoc. Three active sites were identified and the best site was selected on the basis of ligand binding depending on the affinity towards ligand PnPP. These molecular and structural properties of this lipase will help in production of a DAG oil and as a whole it will be helpful in many biotechnological applications.

`Keywords: Lipase, Homology Modelling, Molecular Dynamics Simulations, Docking.