Bioinformatics Approach to Characterization of SGNH/GDSL-hydrolases

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The present analysis is aimed to recognize structural elements of SGNH/GDSL family of enzymes with a novel folding type using bioinformatics tools on data of primary and secondary structures. Out of 770 proteins sequences deposited, data of seven different structures of GDSL hydrolases are solved, only; those of the best resolution were selected among twenty available in PDB (including mutants): rhamnogalacturonan acetyleserase from *Aspergillus aculeatus*, thioesterase I from *E. coli*, platelet-activating factor acetylhydrolase IBγ from *Bos taurus*, platelet-activating factor human acetylhydrolase IBβ, and esterase from *Streptomyces scabies*. Two novel enzymes of our interest, esterase from *Pseudomonas aeruginosa* and lipase from *Streptomyces rimosus*, were included in the analysis and compared with GDSL hydrolases of known three-dimensional structures. These two enzymes were recognized as the members of the SGNH/GDSL family with a fold being different from the common α/β hydrolase fold. Alignment of amino acid sequences of SGNH/GDSL hydrolases studied reveals similarity about 20%. However, four blocks of conserved sequence, with one conserved residue in each block (S,G,N,H) are common characteristics.

Keywords: databases, bioinformatics, novel hydrolase fold