Interaction studies of putative chemical ligands in binding sites of thermostable lipase from Geobacillus zalihae strain T1

ABSTRACT

Industrial biotechnology focusing on the usage of enzyme as the catalyst in many chemical reactions, however enzyme stability remains a major challenge. Enzyme can be modified via genetic or chemical methods by manipulating its structure. A potential biocatalyst based on lipase enzyme was designed by in silico approach. The enzyme-ligand interactions between selected chemical ligands and a thermostable lipase from Geobacillus zalihae strain T1 were studied by using molecular docking, AutoDock 3.0.5. The T1 lipase structure (PDB ID: 2DSN) was predicted to have 65 pockets in the structure, with nine of them have the potential binding sites for ligands based on their surface area, volume and number of residues. The characteristics of each selected binding site and chemical ligands were analyzed. Types of enzyme-ligand interactions involved in binding sites were determined and co-related with the final docked energies. All these discoveries may prove useful for designing novel binding sites, in particular as new biocatalyst.

Keyword: Thermostable lipase; Binding site; Protein-ligand interaction; Docking; Biocatalyst