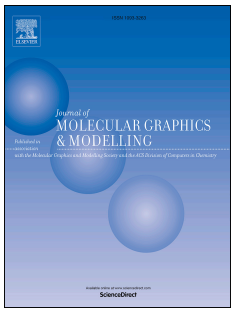
Accepted Manuscript



Understanding domain movements and interactions of *Pseudomonas aeruginosa* lipase with lipid molecule tristearoyl glycerol: A molecular dynamics approach

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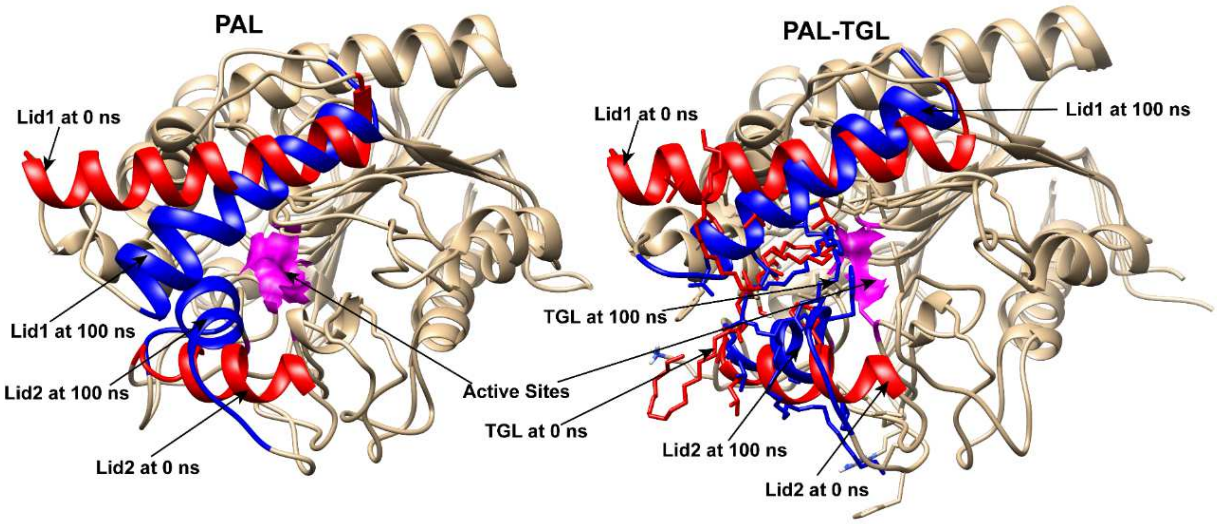
Title:

Understanding Domain Movements and Interactions of *Pseudomonas aeruginosa* lipase with Lipid Molecule tristearoyl glycerol: A Molecular Dynamics Approach

Research Highlights

- Interfacial activation of *Pseudomonas aeruginosa* lipase (PAL) was investigated for 100 ns.
- Lid2 in PAL showed more fluctuations and triggered the movement of lid1 leading to the interfacial activation of PAL in the presence and absence of a lipid molecule tristearoyl glycerol (TGL).



Abstract

Lipases are biocatalysts which exhibit optimal activity at the aqueous-lipid interface. Molecular Dynamics (MD) Simulation studies on lipases have revealed the structural changes occurring in the enzyme, at the loop-helix-loop, often designated as the “lid”, which is responsible for its interfacial activation. In recent years, MD simulation of lipases at molecular level have been studied in detail, whereas very few studies are carried over on its interaction with lipid molecules. Hence, in the current study we have investigated molecular interaction of bacterial lipase (*Pseudomonas aeruginosa* lipase,