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ACCEPTED MANUSCRIPT

The effect of mutations in the lid region of *Thermomyces lanuginosus* lipase on interactions with triglyceride surfaces: a multi-scale simulation study

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Highlights

- Lipases function at the interface between an amphiphilic molecular substrate surface and water
- Molecular simulations reveal interactions of *Thermomyces lanuginosus* lipase (TLL) with a trioleate triglyceride surface
- Wild-type TLL and two variants containing a modified lid region (which covers the active site) were investigated
- Interfacial binding interactions of TLL depend on the nature of the amino acid residues within the lid region
- Our results highlight the role of the dynamic behavior of the lid region in interfacial binding and activation of lipases

Abstract

Lipases naturally function at the interface formed between amphiphilic molecules and the aqueous environment. *Thermomyces lanuginosus* lipase (TLL) is a well-characterised lipase, known to exhibit interfacial activation during which a lid region covering the active site becomes displaced upon interaction with an interface. In this study, we investigate the effect the amino acid sequence of the lid region on interfacial binding and lid dynamics of TLL. Three TLL variants were

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