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## ROLE OF SUBSTRATE BINDING ON THE PROTEIN DYNAMICS OF AN ENDOGLUCANASE FROM FUSARIUM OXYSPORUM AT DIFFERENT TEMPERATURES

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### Abstract

Thermostability is an important requirement for protein function, and one goal of protein engineering is improvement of activity of the enzymes at higher temperatures, particularly for industrial applications. Computational approaches to investigate factors influencing thermostability of proteins are becoming researchers' choice. This study investigates the influence of substrate binding on the protein dynamics by comparing the molecular dynamics simulations of substrate-enzyme complex against un-bound enzyme, using endoglucanase I from *Fusarium oxysporum*. Endoglucanase-substrate complex was prepared by docking and molecular dynamics simulations were carried out at three different temperatures, 313 K, 333 K and 353 K. Our finding shows that the secondary structures for sub state-enzyme complex show more fluctuations relative to un-complexed structure. The same trend was observed for solvent accessible surface area and radius of gyration. At the highest temperature studied (353 K), the substrate-enzyme complex form showed the highest fluctuations. The fluctuations around the active site regions reach a minimum at the optimum temperature, compared to the other structural regions and other temperatures.

### Keywords

**Author Keywords:** [thermostable enzymes](#); [thermostability factors](#); [ligand-enzyme complex](#); [Fusarium oxysporum endoglucanase](#); [molecular dynamics simulations](#)

**KeyWords Plus:** [MOLECULAR-DYNAMICS](#); [THERMOSTABILITY](#); [DOCKING](#)

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