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Type(English)	Outline

Title:

Elucidation of functionally important dynamics and structural changes of the *E. coli* maltose transporter by all-atom molecular dynamics simulations

Outline:

Chapter 1. Introduction

The introduction of the ABC transporter, especially focusing on the *E. coli* maltose transporter ($MalFGK_2E$).

Chapter 2. Analysis of the free energy landscape for the opening-closing dynamics of the maltose transporter ATPase $MalK_2$

In this chapter, I first focused on $MalK_2$ to investigate the relationship between the conformational change and the binding of Mg^{2+}-ATP by performing both conventional all-atom molecular dynamics (cMD) and accelerated molecular dynamics (aMD) simulations. The results indicated that the Mg^{2+}-ATP would facilitate the conformational change from semi-open state to closed state by modifying the free energy surface.

Chapter 3. Molecular dynamics investigation of the full maltose transporter with and without the maltose binding protein MalE

In this chapter, I further performed cMD simulations to examine the full transporter's ($MalFGK_2$ and $MalFGK_2E$) fluctuations and investigated the correlation between each subdomain. The results indicated that the maltose binding protein (MalE) would be the critical subdomain that mediated the protein's fluctuation, and thus facilitate the conformational change from open state to closed state.

Chapter 4. ATP hydrolysis mechanism of the maltose transporter explored by QM/MM metadynamics simulation

In this chapter, I used the QM/MM metadynamics to investigate the ATP hydrolysis reaction in the maltose transporter. I successfully observed the hydrolysis reaction and concluded that this hydrolysis reaction is a one-step, exothermic reaction, and can be described as a one water (1W), dissociative-like, and general base catalysis (GBC) model.

Chapter 5. Conclusion

I have performed an intact investigation for the *E. coli* maltose transporter and proposed an overall model to describe its mechanism.