Contribution ID : **55** Type : **Poster Presentation**

Evaluating free energy landscape of ATP binding and consequent allostery in the helical bundle domain of pRN1 primase

Primases are pivotal for DNA replication. Cellular archaeoeukaryotic primases consist of small catalytic and large accessory domains. The catalytic domain cannot synthesize the primer in the absence of accessory domain, which regulate the function of the primases.Analogously, the catalytic domain (Prim_Pol) of the archaeal plasmid primase (pRN1) is activated by a helical bundle domain (HBD) which promotes the synthesis of the dinucleotide. The DNA replication process is propagated by the binding of the DNA template in a sequence-specific manner in the presence of two ATP molecules bound to the HBD. Thus, the active state of the primase is contingent on binding of the two ATP to the HBD. Recent experimental investigations have revealed that the ATP binding allosterically controls the regulatory role of HBD resulting in a large structural change. Further, even though the binding of two ATP molecules to the HBD is essential for the functioning of the primase, one the ATP is easily exchangeable. Herein, we have carried out atomistic Molecular Dynamics simulations to understand the role of ATP binding and the consequent structural and dynamical effects of the allostery of HBD as well as evaluating the free energies associated with the ATP binding to the HBD using enhanced sampling method.

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