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The Molecular Dynamics Study of the Structural Conversions in the Transformer Protein RfaH JEEVAN GC, BERNARD GERSTMAN, PREM CHAPAGAIN, Florida International University — Recently, a class of multi-domain proteins such as RfaH transcription factor are labelled as the transformer proteins as they undergo major conformational transformation for performing multiple functions. In the absence of the inter-domain contacts, the C-terminal domain of RfaH transforms from its alpha-helix conformation to a beta-barrel structure. Each of these states have their own functional role: in its alpha-helx state, RfaH-CTD inhibits the transcription by masking the binding site of RNAP, but in its beta state it facilitates the translation. We used various molecular dynamics simulations to study its transformer-like behavior of full-RfaH and identified key amino acid residues that are important in modulating such behavior. Our results show that the inter domain interactions constitute the major barrier in the alpha-helix to beta-barrel conversion. Once the interfacial interactions are broken, structural conversion is easier. The structural conversion from beta-barrel to alpha-helix proceeds with the rearrangement of the hydrophobic residues followed by the inter domain contacts formation via non-native, transient salt-bridge formation, leading to the formation of the native inter domain salt-bridge and hydrophobic contacts to give the final alpha-helix structure.

Jeevan GC
Florida International University

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