Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Molecular Dynamics Investigations of the alpha-helix to Beta-barrel Conformational Transformation in RfaH JEEVAN GC, YUBA BHANDARI, BERNARD GERSTMAN, PREM CHAPAGAIN, Florida International University — We used combination of replica exchange molecular dynamics simulations with implicit solvent and detailed all-atom simulations with explicit solvent to investigate the α-helix to β-structure transformation of RfaH-CTD. While interacting with the N-terminal domain (NTD), the C-terminal domain (CTD) of RfaH folds to a α-helix bundle but it undergoes an all-α to all-β conformational transformation when it does not interact with the NTD. The RfaH-CTD in the all-α topology is involved in regulating transcription whereas in the all-β topology it is involved in stimulating translation by recruiting a ribosome to an mRNA. Calculations of free-energy landscape and transfer entropy elucidate the details of the RfaH-CTD transformation process. The importance of interfacial interactions between the two domains of RfaH is highlighted by the compromised structural integrity of the helical form of the CTD in the absence NTD. We also studied interdomain and intradomain interactions in RfaH using Steered Molecular Dynamics Simulations. We investigated the role of the interdomain salt-bridge interaction in the domain stability Potential mean force was calculated to obtain free energy profile using Jarzynski Equality.

Jeevan Gc
Florida Intl Univ

Date submitted: 14 Nov 2014 Electronic form version 1.4