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Computational Study on the Dynamics and Structural Conversion of RfaH JEEVAN GC, BERNARD GERSTMAN, PREM CHAPAGAIN, Florida International University — RfaH undergoes major structural rearrangements to perform multiple functions. The C-terminal domain (CTD) of RfaH showed that it can exist as either an α-helix bundle when interacting with the N-terminal domain (NTD), or as a β-barrel conformation when it is not interacting with the NTD. They perform different functions in these states and hence are labeled as "Transformer Proteins". We investigate the full RfaH using a variety of all-atom Molecular Dynamics (MD) simulation techniques. We find that the CTD-NTD domain-domain interactions constitute the major barrier in the CTD α-helix to β-barrel structural conversion. The structural transformation of the CTD is relatively easy after the detachment of inter domain interactions. We pointed out important amino acids residues that play especially important roles in controlling the inter-domain motions.

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