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Structure and dynamics of Ebola virus matrix protein VP40 by a coarse-grained Monte Carlo simulation RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Ebola virus matrix protein VP40 (consisting of 326 residues) plays a critical role in viral assembly and its functions such as regulation of viral transcription, packaging, and budding of mature virions into the plasma membrane of infected cells. How does the protein VP40 go through structural evolution during the viral life cycle remains an open question? Using a coarse-grained Monte Carlo simulation we investigate the structural evolution of VP40 as a function of temperature with the input of a knowledge-based residue-residue interaction. A number local and global physical quantities (e.g. mobility profile, contact map, radius of gyration, structure factor) are analyzed with our large-scale simulations. Our preliminary data show that the structure of the protein evolves through different state with well-defined morphologies which can be identified and quantified via a detailed analysis of structure factor.

Ras Pandey
University of Southern Mississippi

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