Abstract Submitted
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Study on the Dynamics of Influenza Hemagglutinin Based on Energy Landscape Theory[1] XINGCHENG LIN, NATHANIAL EDDY, JEFFREY NOEL, Rice University, PAUL WHITFORD, Northeastern University, JIANPENG MA, Baylor College of Medicine, JOSE ONUCHIC, Rice University — Hemagglutinin (HA2), a homotrimeric influenza surface protein crucial for membrane fusion, undergoes an drastic structural rearrangement during viral invasion of the host. X-ray crystallography shows that the pre- and post-fusion configurations have largely disparate secondary, tertiary and quaternary structures. Simulations allow us to explore the time-dependent high resolution structural information and function of HA2 dynamics. Here we use an approach based on energy landscape theory that combines the native information from both the starting and end points. Our simulation shows two key events in the conformational transition of HA2: The extension of its fusion peptides away from the viral membrane and the melting of its globular C-terminal portion. The similar timescale and a kinetic competition between these two events lead to two main pathways and generic kinetic intermediates during this transition. Through considering the biological context of HA, we test perturbations of the baseline model that are useful in understanding the robustness of our predictions and how they translate into the function of HA. The all-atom explicit solvent simulation is performed and convince the cracking phenomenon at the start of this protein dynamics.

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