Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Molecular Dynamics of the ZIKA Virus NS3 Helicase BRYAN RAUBENOLT, STEVEN RICK, Univ of New Orleans, THE RICK GROUP TEAM — The recent outbreaks of the ZIKA virus (ZIKV) and its connection to microcephaly in newborns has raised its awareness as a global threat and many scientific research efforts are currently underway in attempt to create a vaccine. Molecular Dynamics is a powerful method of investigating the physical behavior of protein complexes. ZIKV is comprised of 3 structural and 7 nonstructural proteins. The NS3 helicase protein appears to play a significant role in the replication complex and its inhibition could be a crucial source of antiviral drug design. This research primarily focuses on studying the structural dynamics, over the course of few hundred nanoseconds, of NS3 helicase in the free state, as well as in complex form with human ssRNA, ATP, and an analogue of GTP. RMSD and RMSF plots of each simulation will provide details on the forces involved in the overall stability of the active and inactive states. Furthermore, free energy calculations on a per residue level will reveal the most interactive residues between states and ultimately the primary driving force behind these interactions. Together these analyses will provide highly relevant information on the binding surface chemistry and thus serve as the basis for potential drug design.

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Date submitted: 11 Nov 2016 Electronic form version 1.4