Title: Protein aggregation and protein-membrane interactions of the matrix (MA) domain of HIV-1 Gag protein

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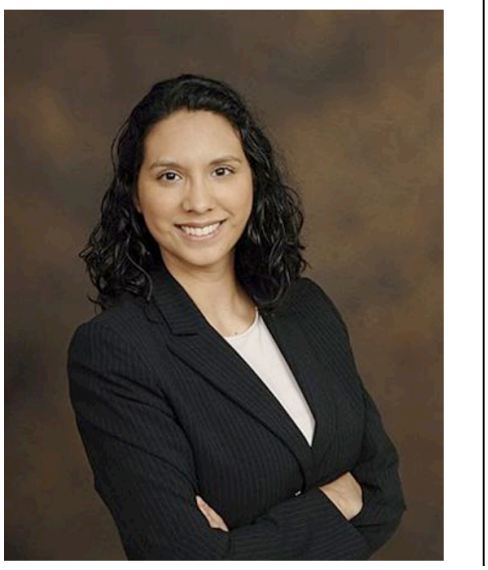
Abstract

Binding and aggregation of the HIV-1 Gag protein to the plasma membrane (PM) enable budding and release of immature virions, which enable the propagation of viral infection. The matrix (MA) domain of the Gag protein is a 131-amino-acid sequence responsible for targeting the membrane. The MA domain seems to favor electrostatic interactions at the membrane surface in places where PIP_2 lipids are more abundant. The myristate group (Myr), a fatty acid covalently attached to the N-terminus of the protein, serves as an anchor once initial binding occurs. The mechanism of Myr release from its binding pocket and its insertion into the membrane is still unclear. NMR studies suggest MA trimerization facilitates Myr exposure from its sequestered conformation, leading to Myr anchoring. Using molecular dynamics and enhanced sampling techniques, such as metadynamics, we examined MA-membrane interactions with model membranes for the PM as well as MA-MA interaction and trimerization. We looked at the effect of lipid composition, specifically the presence of PIP_2 and cholesterol, on MA binding events and whether membrane-binding promotes lipid reorganization and raft formation. We present the protein conformational changes that take place during Myr exposure, MA-membrane binding, and MA trimerization. Computational resources for this work were available through XSEDE (Stampede2 and Bridges) and the Anton2 machine from the Pittsburgh Supercomputing Center.

Biography

Viviana M. completed her PhD at the age of 28 from the University of Maryland-College Park, USA. She is currently a postdoctoral scholar at the Voth Lab in the Chemistry Department at the University of Chicago. She has 10 publications, 3 as first author, and 4 more under preparation. Viviana contributed with over 10 posters and oral presentations at multiple conferences and simposia since 2013, both in the USA as well as abroad. She was born in Barcelona, Spain and grew up in Bolivia, where she has also presented her work as invited speaker at the "Universidad Mayor de San Andres" in seminar series prepared by the departments of Physics and Chemical Engineering and the IBTEN (the national regulatory institution of nuclear energy in Bolivia).

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