Virion channel proteins – self-assembly and ion dynamic

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Abstract:

The genomes of many viruses encode short membrane proteins which are known to self-assemble and, consequently, to increase the permeability of lipid membranes for ions and small substrates. The same protein also uses protein – protein interactions (PPIs) to manipulate the mechanism of function of membrane proteins of the host. Structural and mechanistic features of how these viral proteins accomplish their roles are still to be elucidated. PPIs with host proteins serve as valuable template for drug development.

Biological relevant features are investigated using two computational platform technologies which cover different time and size scales: coarse grained and classical molecular dynamics (MD) simulations. With these techniques (i) assembly of the proteins and (ii) mechanics of gating are investigated for bitopic Vpu of HIV-1 and polytopic p7 of HCV, respectively. For Vpu, distinct binding modes upon dimerization and oligomerization of the protein are observed. Simulations of p7 reveal mechanical features of the TMDs as well as rectified ion dynamics.

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