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# Virion ion channels – energetics involved in short-circuiting the lipid membrane.

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Lipid membranes are impermeable dielectric barriers for charged particles being able to store electrical energy which can be used for biological processes. Proteins embedded in the lipid membrane lower the barrier by enabling the formation of aqueous pores. Ions can flow across the membrane along a concentration gradient through these pores, a process which is equivalent to short-circuit. How the proteins assemble forming pores is not known as well as how ion flux is supported by the mechanics of the protein. Computational techniques such as molecular dynamics simulations play an important role in making suggestions.

Virion ion channel forming proteins (VCPs) are encoded by many viruses supporting the infectivity cycle of the virus. Due to their small size they can be seen as miniaturized ion channels and serving as templates for the generation of ion channels *per se*. Insights into protein and ion dynamics of the polytopic VCP p7 of hepatitis C virus (HCV) with two transmembrane domains (TMDs) are presented using several force fields. The energy of ions within the pore of assembled bitopic 8a of severe acute respiratory syndrome corona virus (SARS-CoV) on the basis of potential of mean force (PMF) calculations is assessed. While the ions in 8a experience energy barriers of ~2 kcal/mol, they can reach up to 15 kcal/mol in an analog structural model of a human ion channel. These values are lower than binding energies of soluble proteins which can reach ~40 kcal/mol.

**Keywords**: Virion ion channels, ion permeation, protein mechanics, potential of mean force, molecular dynamics simulations.