Lipid specificity of Viral Fusion Proteins

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Viral fusion proteins drive fusion of viral and host cell membranes in a series of complex structural transition events. Although the structure of several fusion proteins has been solved, the characterization of viral protein-membrane interactions at atomistic resolution is still missing. Membrane interactions of fusion proteins are conserved and occur via fusion peptides (FPs) in class I and fusion loops (FLs) in class II/III proteins. Previously, we had characterized the glycerophospholipid binding in class II fusion protein glycoprotein C (gC) of Rift Valley fever virus (RVFV) [2] and the studies revealed specific binding pocket for PC lipid. Here we aim to understand if specific lipid binding site also exists in class I and III viral fusion proteins and dependence of lipid headgroup type, tail length and degree of lipid tail unsaturation for protein binding. Molecular dynamics (MD) simulations is an excellent technique to understand how proteins associates with lipid membrane at atomistic resolution and here we make use of MD simulations to gain structural insights into lipid contact sites and membrane insertion of FP / FL residues.

[1] M. Vallbracht et al., J Virol 92: e01203-17, (2018)
[2] P. Guardado-Calvo et al., Science 358, 663-667, (2017)