Lipid specificity of the glycoprotein B of pseudorabies virus

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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 membrane fusion mechanism at atomistic resolution is still missing. Recently, glycoprotein B (gB) ectodomain of pseudorabies virus (PrV) was resolved and the structure adopts a typical class III postfusion trimer conformation [1], however, the interactions with the membrane was not well established. 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 in this study we aim to understand if class III protein are anchored to the membrane by specific lipid binding pockets as found for RVFV. Molecular dynamics (MD) simulations is an excellent technique to understand how gB associates with lipid membrane at atomistic resolution, thus providing structural insights into lipid contact sites and membrane insertion depth of FL residues.

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