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Coronavirus Envelope Protein: Lipid Sensitivity and Membrane Bending JESSE SANDBERG[1], GRACE BRANNIGAN[2], Rutgers University, Camden — The Coronavirus envelope (E) protein is a pentameric viroporin that is implicated in numerous viral processes including but not limited to assembly, budding, envelope formation, and pathogenesis. While much work has recently been done to characterize this protein's structure, function, and interactions with other proteins, its interactions with and effects on surrounding membranes are less well understood. It is known that the viroporin loses ion-selectivity in an exclusively neutral lipid environment, but it is not clear what drives this behavior. In the present study we use coarse-grain molecular dynamics (CG-MD) simulations to identify stable binding sites for anionic lipid headgroups. We then use all-atomistic molecular dynamics simulations to investigate the effect of lipid charge on viroporin structure using the sites identified from CG-MD. The E protein also induces membrane curvature, although the precise mechanism is unknown. Using CG-MD, we observe that the E protein bends the membrane in simulations with lipid species that have long acyl chains. We find this effect is limited when shorter lipid species are used, which suggests it results from asymmetric mismatch between the viroporin transmembrane domain and the thickness of a typical host membrane.

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