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Interaction of SARS-CoV-2 Fusion Peptides with Lipid Monolayers by Molecular Dynamics Simulations

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Membrane fusion between the viral envelope and host cell is a key stage during the infectivity of SARS-CoV-2 that enables the release of the viral genetic material into the target cell. Within the region of the Spike protein implicated in this process, several peptides have been identified to interact with the cell membrane [1]. Through Molecular Dynamics (MD) simulations, we aim to elucidate the role of these fusion peptides in viral infection by investigating their interactions with biomimetic model membranes, using lipid monolayers to represent a membrane leaflet. We first use all-atom (AA) MD simulations to obtain a stable conformation for each peptide in physiological conditions. The resulting structures are then mapped into a coarse-grained (CG) model in order to increase the length and timescales for the studied systems. The CG model we employ, Martini 2, developed to simulate the behavior of a lipid membranes [2] and proteins [3], has been proven to be transferable to a wide range of biological systems [4]. We explore the effect that each peptide has on the interaction with biomimetic lipid monolayers under varying surface area as well as how lipid composition affects their binding to the membrane.

References
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