Molecular Dynamics Simulations Shed Light on Antimicrobial Peptide Interactions with COVID-19 Altered Membranes

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In recent years, the COVID pandemic has garnered a great deal of attention, focusing mainly on the acute phase of the disease. However, this is only the beginning, as some patients continue to experience persistent symptoms, known as Post-COVID Condition (PCC), and an estimated 20% of those affected do not recover.[1,2] The presence of this condition shows a number of obstacles, including the lack of suitable therapeutic options and the long-term consequences for survivors of the disease.

While the study of genome sequencing and the protein composition of the virus membrane is of undeniable value for vaccine development, there are other aspects that have been overlooked. One of these is the lipid profile of patients with COVID-19. The lipid profile plays a crucial role not only during the acute phase, but also throughout disease progression and during medium- and long-term effects[3,4]. There appears to be a potential connection between the lipid profile and COVID-19, suggesting that the innate immune system, specifically antimicrobial peptides (AMPs), may be responsible for this association[5]. Therefore, understanding the importance of the lipid profile and how AMPs function at the interface of lipid membranes affected by COVID-19 could improve our understanding of the disease and potentially contribute to the development of better treatments.

To investigate the interaction between antimicrobial peptides and infection-affected membranes, we performed Molecular Dynamics (MD) simulations with various AMPs and models of altered and unaltered membranes. The findings of this study may provide deeper insight into the role of AMPs in the lipid profile of patients with COVID-19 and PCC, which could lead to the development of more effective treatments.

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