Structural Changes of the SARS CoV-2 Spike Protein in Varying Salt Concentrations

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Previous studies have uncovered the structure of the SARS-CoV-2 spike glycoprotein, which plays a key role in cell membrane fusion. In addition, it has been shown that the ion concentration of a solution can have significant effects on protein behavior. The SARS-CoV-2 virus is primarily transmitted through respiratory droplets, which increase in salt concentration as their water content evaporates over time. Therefore, the aim of this study is to simulate the SARS-CoV-2 spike glycoprotein in NaCl concentrations corresponding to those found in drying saline droplets to determine whether the saline levels will cause significant structural changes or denaturation in the protein. Simulations of the protein in a water box were run using GROMACS molecular dynamics software, and NaCl concentrations of 0M, 0.5M, 1M, and 1.5M were used. Then, the values for RMSD and SASA were extracted over time. The time series for these variables were compared across different concentrations to determine if any significant trends or differences occurred. The conclusion of this study is that there were no significant changes in the protein structure when comparing varying salt concentrations, indicating that the spike glycoprotein is tolerant to high salt concentrations and may even be halophilic. This implies that the SARS-CoV-2 virus in a drying respiratory droplet on a contaminated surface may retain its viral viability even as the salinity of the droplet increases over time.

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