Title:	Drug repurposing and sequence analysis in S-glycoprotein variants reveals critical signature patterns and destabilization of receptor-binding domain in omicron variant
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Abstract:	The evolution of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) virus since its emergence in 2019 has yielded several new viral variants with varied infectivity, disease severity, and antigenicity. Although most mutations are expected to be relatively neutral, mutations at the Spike region of the genome have shown to have a major impact on the viral transmission and infection in humans. Therefore, it is crucial to survey the structures of spike protein across the global virus population to contextualize the rate of therapeutic success against these variants. In this study, high-frequency mutational variants from different geographic regions were pooled in order to study the structural evolution of the spike protein through drug docking and MD simulations. We investigated the mutational burden in the spike subregions and have observed that the different variants harbour unique signature patterns in the spike subregions, with certain domains being highly prone to mutations. Further, the MD simulations and docking study revealed that different variants show differential stability when docked for the same set of drug targets. This work sheds light on the mutational burden and the stability landscape of the spike protein across the variants from different geographical regions.
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