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Drug repurposing: molecular modelling

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Measures to combat SARS-CoV-2 infection include the development of antiviral agents as well as the repurposing of existing drugs targeting key stages of the viral life cycle. Viral entry occurs through the interaction of the spike protein with host cell receptors and its subsequent proteolytic activation by host proteases. Identification of host cellular factors exploited during viral entry, replication, and activation enables the discovery of novel therapeutic targets. Molecular docking was employed to evaluate the binding affinity of pharmaceutical compounds to SARS-CoV-2 proteins, with particular emphasis on potential inhibitors of the furin protease and the impact of spike protein mutations on drug–protein interactions. Docking assesses the energetic favorability of ligand–target binding and supports early-stage drug repurposing. To further refine complex stability and structural features, molecular dynamics simulations were performed under physiologically relevant conditions, including explicit solvent, ions, and temperature control. Overall, our results confirm that computational modeling is an effective tool for virtual screening in antiviral drug repurposing.

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