High Throughput Virtual Screening for the Identification of Potent Inhibitors of SARS-CoV-2 Spike Protein

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In this work, we focused on the discovery of potential compounds that could obstruct the binding of the SARS-CoV-2 spike protein to human angiotensin-converting enzyme 2 (hACE2). We performed a structure-based virtual screening including non-covalent molecular docking, molecular dynamics simulations, absolute binding energy calculations, and steered molecular dynamics to study the relative stability of the protein–ligand interactions. This study provides useful insights into the *de novo* design of high-affinity ligands that could thwart the binding of the viral spike to the human ACE2 protein.