A Molecular Docking Study Repurposes FDA Approved Iron Oxide Nanoparticles to Treat and Control COVID-19 Infection

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Abstract

COVID-19, is a disease resulting from the SARS-CoV-2 global pandemic. Due to the current global emergency and the length of time required to develop specific antiviral agent(s) and a vaccine for SARS-CoV-2, the world health organization (WHO) adopted the strategy of repurposing existing medications to treat COVID-19. Iron oxide nanoparticles (IONPs) were previously approved by the US food and drug administration (FDA) for anemia treatment and studies have also demonstrated its antiviral activity in vitro. Therefore, we performed a docking study to explore the interaction of IONPs (Fe2O3 and Fe3O4) with the spike protein receptor binding domain (S1-RBD) of SARS-CoV-2 that is required for virus attachment to the host cell receptors. A similar docking analysis was also performed with hepatitis C virus (HCV) glycoproteins E1 and E2. These studies revealed that both Fe2O3 and Fe3O4 interacted efficiently with the SARS-CoV-2 S1-RBD and to HCV glycoproteins, E1 and E2. Fe3O4 formed a more stable complex with S1-RBD whereas Fe2O3 favored HCV E1 and E2. These interactions of IONPs are expected to be associated with viral proteins conformational changes and hence, viral inactivation. Therefore, we recommend FDA-approved-IONPs to proceed for COVID-19 treatment clinical trials.

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