Molecular docking studies of silver nanoparticles (AgNPs) for their potential use against SARS-CoV-2

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Abstract

Comprehending the COVID-19 pandemic and preventing future coronavirus pandemics hinges on our ability to grasp the evolutionary strategies employed by the SARS-CoV-2 Omicron variant. In the present investigation, we determined the crystal structure of the receptor-binding domain (RBD) from currently circulating omicron subvariant XBB.1.5 complexed with silver nanoparticles AgNPs. The primary function of the spike protein RBD is to bind to the receptor angiotensin-converting enzyme 2 human cellular receptor (hACE2) that helps the virus enter the host cell . The docking studies revealed that AgNPs have the capacity to bind to the spike protein RBD, potentially elucidating their antiviral effects against SARS-CoV-2 . Obtained results showed a favorable binding energy of -10.2 Kcal/mol between the nanoparticles and the protein target. According to the docking analysis, AgNPs formed four bonds at the binding site, three hydrogen bond between ALA153 of spike protein and Ag atom, and one σ bonds between LEU281 of spike protein and Ag atom, underscoring their interaction with the active site. AgNPs exhibit potential as effective agents against viruses raising the possibility of their use in the treatment and prevention of COVID-19 and used to develop effective antiviral drugs.

Keywords: *Green synthesis; Silver nanoparticle; Molecular docking*.