A Computational Study on Gold and Silver Nanoparticles Against SARS-CoV-2 Proteins

Ilyes Zatla [1],* & Lamia Boublenza[1]

[1] Laboratory of Microbiology applied to the Food industry, Biomedical and the Environment, Faculty of Natural and Life Sciences, Earth and Universe Sciences. Department of Biology. University of Tlemcen, Algeria.

*** Author for correspondence:** E-mail: ilyes.zatla@univ-tlemcen.dz, Tel: +213-540-315422

Abstract

Metallic nanoparticles, such as gold and silver nanoparticles, are extraordinarily small particles composed of metal atoms at the nanoscale, typically ranging in size from 1 to 100 nanometers. These nanoparticles possess a plethora of unique and invaluable properties owing to their diminutive size, exceptionally high surface area-to-volume ratio, and the emergence of quantum effects at this scale. In this research, a computational simulation was conducted to explore the structural configurations of both silver nanoparticles (AgNPs) and gold nanoparticles (AuNPs). Subsequently, geometry optimization techniques were applied to refine these structures. The optimized nanoparticle configurations were then systematically evaluated for their potential interactions with three specific targets within the SARS-CoV-2 virus: the Main protease (Mpro), RNA-dependent RNA polymerase (RdRp), and the S spike glycoprotein. Notably, the results revealed that both AgNPs and AuNPs exhibited remarkable affinities for the active pockets of SARS-CoV-2 Mpro, suggesting their potential utility as inhibitors for this critical viral protein. Intriguingly, when considering RdRp, AgNPs displayed superior binding affinity compared to AuNPs, indicating their specific potential in targeting this component of the virus. Conversely, when assessing their interactions with the S spike glycoprotein, AuNPs demonstrated greater binding affinities than AgNPs, with more pocket residues being involved in this interaction. The versatility of gold and silver nanoparticles extends far beyond virology, as these materials find applications in diverse fields, including medicine, electronics, and environmental remediation. The findings presented here underscore their potential as versatile antiviral agents, providing a promising avenue for further in vitro and in vivo research to explore their efficacy in inhibiting the replication of the SARS-CoV-2 virus.

Key words: SARS-CoV-2, COVID-19, Anti-virals, Nano-particles, Molecular dynamics.