Impact of magnesium, zinc, selenium, copper, and iodine food supplements on SARS-CoV, SARS-CoV-2 viruses and their adducts with human ACE2 enzyme: A Computational Based Investigation

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Abstract

In a search for drugs of the potential impact on SARS-CoV and SARS-CoV-2, we have chosen different forms of metal-based food supplements to investigate. We computed their binding to specific peptide sequences of the spike virus S-protein: angiotensin-converting enzyme 2 (ACE2) interface-drug binding adduct. Manual docking was applied. The chosen molecules located themselves to achieve minimum energy geometries, resulting in limiting the viral recognition of the host cells or disturbing the host-virus interactions. Based on the HOMO ό"LUMO frontier orbitals, we successfully used the computed reactivity indices to explain the simulation results. The results are compared with that similarly simulated interactions between the protein/protein and the experimentally allowed remdesivir drug that has been granted emergency use authorization by the FDA. These computationally based findings also suggest that the simple computational indices and methods could point to promising medicines to help with the fight against COVID-19. However, in vivo and in vitro, experimental validation is now required.