A COMPUTATIONAL APPROACH TO ESTABLISH AND ROGRAPANIN AS A POTENT STRUCTURAL IN HIBITOR OF M^{PRO} OF SARS-COV-2

DIJENDRA NATH ROY

Assistant Professor, Department of Biotechnology, National Institute of Technology-Raipur, Raipur, Chhattisgarh, PIN-492010, India
E-mail: dnroy.bt@nitrr.ac.in

Coronavirus disease (COVID-19) is an infectious disease caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) virus. Most people infected with the virus have experienced mild to moderate respiratory illness. According to the World Health Organization (WHO), the rate of infection and rate of mortality caused a global pandemic that led to a dramatic loss of human life worldwide to date. Due to the absence of any effective antiviral drug to treat COVID-19 infection, its lethality is severe and worst. The main protease of SARS-CoV-2, M^{pro} is considered one of the potential drug targets because of its role in the processing of proteins translated from viral RNA. In this report, four of the plant metabolites, 14-deoxy-11,12-didehydroandrographolide, andrograpanin, quinine, and cinchonine from two eminent medicinal plants Andrographis paniculata and Cinchona officinalis, have been evaluated against the main protease M^{pro} of SARS-CoV-2 by applying in-silico molecular docking and molecular dynamics simulations. These four compounds have been chosen for their antimicrobial activity against many infectious diseases. Here, it is found that the andrograpanin has a strong binding affinity with the target protein in its active site with potential negative energies. The studies using Molecular Dynamic Simulation (MDS) and Molecular Mechanics with Generalized Born and Surface Area Solvation (MM/GBSA) suggest that andrograpanin exhibits effective binding interactions involving identical amino acid residues with the same binding pockets of the main protease of SARS-CoV-2 like earlier reported N3 inhibitor. Therefore, these theoretical experiments suggest that the andrograpanin could be a promising inhibitor against M^{pro} present in SARS-CoV-2, which leads to eradicating the COVID infection.

Keyword - SARS-CoV-2; Virus; Andrograpanin; COVID-19; Drug Target; Infection