

International Conference on Chronic Infectious Diseases and Vaccinations (ICCIDV 2025)

Conference Proceedings

February 06, 2025 - Singapore

Careful Investigation of Some Biomolecules That Might Be Successful in Preventing Sars-Cov-2/COVID-19 Using In-Silico Analysis: Preliminary Research

Dr. Rahul Hajare

Sandip University, School of Pharmaceutical Science, Nashik, India

In 2019, the corona virus (SARS-CoV-2) with highly contagious features caused millions of cases worldwide. Scientists now feel more pressure than ever to create a unique cure. Due to the strong spreading properties that increased the death rate, medical professionals administered Remdesivir, dexamethasone, azithromycin, and hydroxychloroquine, among other treatments. An alternative Ayurvedic treatment that is safe and has no side effects can be helpful, even though a medication has now been licensed and vaccinations have been given to combat the symptoms. Because these plants are endowed with strong chemical contents, this study is focused on a selection of prospective plants. According to a review of the literature, these chemical components support the body's defenses against illness, lower inflammation, supply antioxidants, and increase resistance. Consequently, the protein crystalline structure of SARS-CoV-2 Mpro was carried out in the current study, In-silico analysis of selected markers against 6LU7. The average binding energy of the following compounds was determined: -5.67, -6.01, -6.47, -6.41, -6.92, -6.52, -6.35, -6.47, -6.98, -6.83, -6.52, -7.86, -6.36 kcal/mol for nobiletin, tangeretin, sideroxylonal C, Coriandron, Epicatechin, epigallocatechin gallate, luteolin, Ombuin, Tamarixetin, 6-deacetylnimbin, nimbolide, and Tricin, respectively. Furthermore, nine bioactive markers, namely PHE140, CYS145, GLU166, GLN189, Epicatechin, Nobiletin, Tamarixetin, Ombuin, and nimbolide, exhibit comparable binding active sites with the synthetic drug Remdesivir. Additionally, binding energy scores, binding affinity, and ADMET modeling are the main topics of the inquiry. Nonetheless, immunization is a necessary condition to stop the spread of infection.