Indian Journal of Chemistry
Vol. 62, December 2023, pp. 1252-1267
DOI: 10.56042/ijc.v62i12.5525

Virtual screening and molecular docking study of some naturally available phytochemicals against SARS-CoV-2

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Received 14 August 2023; accepted(revised) 24 November 2023

The novel human corona virus disease 2019, also known as COVID 19 or SARS-CoV-2 has designated as severe acute respiratory syndrome coronavirus 2, which has first emerged in Wuhan, China at the end of 2019. Now a day, it is a great challenge to scientists in the area of biology and chemistry to develop anticoronaviral drugs to overcome from this disease. SARS-CoV-2 was identified as a single-stranded positive-sense RNA virus. In this study, we have used virtual screening and molecular docking investigation of some naturally occurring bioactive organic compounds having the various phytochemical properties to compare the potential inhibitory activity of these molecules against SARS-CoV-2 protease. Based on ADME analysis and molecular docking study, Amentoflavone, Kazinol A, Kazinol B, Berbamine, Broussoflavan A, (-)-Catechingallate and Juglanin exhibits remarkable potentiality to bind with M^{pro} as compared to native ligand N3. Moreover the bioavailability radar study shows that Broussoflavan A is the only compound which is orally bioavailable among the studied compounds. A molecular dynamics simulation study of the ligand (Broussoflavan A) with protein indicates that the complex is stable. The docking study and MD simulation study indicates that in the protein-ligand complex, Broussoflavan A interact with active site of SARS-CoV-2 main protease.

Keywords: Naturally Available Phytochemicals, Virtual Screening, Molecular Docking, MD-Simulation