

Title: Identification of new inhibitors for the avian H1N1 virus through molecular docking and dynamic simulation approaches

Author: Md Rezaul Islam, Shankar Sharma, Sk Yeasir Arafat, Rahul Dev Bairagi, Jehad Zuhair Tayyeb, Imren Bayıl, Gabriel Christian de Farias Morais, Magda H Abdellattif, GUENDOUZI Abdelkrim, Jonas Ivan Nobre Oliveira

Abstract: The new variant of influenza A virus is known as avian H1N1 subtype which particularly affects birds, and poultry. However, recently it is affecting in human, and creating global health problem. So, this research has studied the myricetin derivatives as novel therapeutic agents that target the Hemagglutinin Protein in Avian H1N1 Virus. The study is focused on addressing the critical need for effective antiviral agents through computational drug design approaches. The research assesses the binding affinities, quantum calculation, molecular dynamic simulation, binding free energy calculation, electronic characteristics, DCCM, PCA and stability of myricetin derivatives with the hemagglutinin protein. This extensive investigation has documented that all the compounds showed outstanding binding affinities, more precisely compounds like 03 and 47, which show better binding energies than the conventional antiviral Tamiflu. Furthermore, the reactivity, pharmacokinetics, and stability, molecular dynamics simulations, ADMET characteristics, and quantum chemical descriptors are investigated, and they all are satisfied by favorable drug like properties. Besides that, this research highlights the significance of electrical characteristics, dipole moment, and hydrogen bonding in developing efficient antiviral medications. In addition, the myricetin derivatives show promise for oral delivery based on ADMET (absorption, distribution, metabolism, excretion, and toxicity) characteristics. Finally, the molecular dynamics simulations show that the ligand-protein complexes are stable and flexible over the MD simulation of 100 ns. Although, the discovered compounds show potential interactions with the avian H1N1 influenza A virus, with outstanding binding affinity, however, it is still crucial needed to perform experimental validation in near future.

Keywords: Avian H1N1 influenza, Hemagglutinin protein, Myricetin derivatives, Computational drug design, Molecular docking, Binding affinity

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