Acta Scientific Pharmaceutical Sciences (ISSN: 2581-5423)

Volume 4 Issue 8 August 2020

Short Communication

Natural Compounds against the Main Protease (Mpro) SARS-CoV-2 through *In Silico* Approach

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DOI: 10.31080/ASPS.2020.04.0565

Received: June 25, 2020

Published: July 18, 2020

Currently, coronaviruses are contagious pathogens and primarily responsible for respiratory and intestinal infections (RIIs). Research on progress to develop antiviral agents (AVAs) against these coronavirus. Researcher had been demonstrated that the main protease (Mpro) protein may represents an effective drug target (EDT) [1]. The novel Corona-virus (n-CoV), recently called as the severe acute respiratory syndrome coronavirus (SARS-CoV-2). The need of the hour is required progress on research into drugs to treat this infection. SARS-CoV-2 remains essential in several research laboratories among the both (national and international).

Natural herbal remedies (NHRs) have long been associated with the oral tradition for treating illnesses. Modern medicine has potential effects thanks to traditional medicine, the effectiveness of which derives from medicinal plants including with herbs and shrubs [2]. Objectively this study is to determine the components of the natural origin compounds (NOCs) have an anti-viral effect (AVE) and capable to prevent the humans from viral infection SARS-CoV-2. This coronavirus SARS-CoV-2 is using the most reliable method is suitable for molecular docking. We used to find out the interaction study between the molecules and the protein. In our study based on the inhibitor of Coronavirus (nCoV-2019) main protease enzyme. We performed *in silico* method for screening of all the compounds from *Curcuma longa L.* (*Zingiberaceae* family) against Mpro protein inhibition.

Coronaviruses are a group of RNA viruses that causes diseases among mammals and birds. This viruses are constituting with very non-segmented positive-sense single-stranded RNA viruses (NSPSSSRVs), which are the important part of the family Coronaviridae. Researcher distributed in humans [3] and the subfamily Orthocoronavirinae, order *Nidovirales*, and realm *Riboviria*.

According to the centers for disease control and prevention (2020), there are major seven types of genera in the coronaviruses are 229E (alpha coronavirus), NL63 (α coronavirus), OC43 (β coronavirus), HKU1 (β coronavirus), MERS-CoV (the β coronavirus that causes Middle East Respiratory Syndrome (MERS), SARS-CoV (the β coronavirus that causes severe acute respiratory syndrome, or SARS and SARS-CoV-2 (the novel coronavirus that causes coronavirus disease 2019, or nCoV-19) [4]. In humans, these viruses are the causal factor of the respiratory tract infections (RTIs) that ranges from mild to the lethal category. Mild illnesses are noticed with new cases of the common cold and throat infections.

Although, two zoonotic coronaviruses are located in the Middle East Respiratory Syndrome Coronavirus (MERS-CoV) and Severe Acute Respiratory Syndrome Coronavirus (SARS-CoV) which viruses are especially affect to the respiratory system through serious infections. The major characteristics of this group is production effects (PEs), nosocomial transmission (NCT), replication in the lower respiratory tract (LRT), and viral immunopathology (VIP). MERS-CoV and SARS-CoV is obtaining from the serious public health problems (SPHPs) lead to epidemics resulting in significant loss of the life values ultimately [5].

Additionally, these two zoonotic coronaviruses (Z-CoV) are infecting among pregnant women. They may misleads to very poor obstetric outcomes as currently no specific vaccine treatment approved for coronavirus infection [4]. As per the causal factor concerned fever, cough, fatigue, production of sputum (POS), shortness

of breath(SOB), sore throat, headache, reports of diarrhea (ROD), vomiting and pneumonia should not be avoided. Researcher identified that β- coronavirus in Wuhan, Hubei Province in China [6]. Firstly, β- coronavirus named as 2019- novel coronavirus (2019-nCoV) on 12 January 2020.

WHO formally named the disease as coronavirus 2019 (COVID- 19). As per the world emergency disease (WED) of cause and concern globally. International Committee of Coronavirus Study Group (ICCSG) had been recommended that use of the name as SARS- CoV-2 on 11 February 2020. Bat was suspected as the natural host of the virus analyzing through the pattern of viral sequences (POVSs) and the pattern of evolutionary sequence analysis (POESA) [7]. The results we obtained from molecular docking shown that among 235 molecules of natural origin. Sixteen molecules are the best compounds observed through molecular docking and hydrogen bonding with interaction (Curcumin (curcumin I; 1-(4-hydroxy-3-methoxyphenyl)-7-(3, 4-dihydroxyphenyl)-1, 6-heptadiene-3, 5-dione; Tetrahydroxycurcumin; 1,5-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-4,6-heptadiene-3-one; Cyclocurcumin; 1-(4-hydroxy-3-methoxyphenyl)-5-(4-hydroxyphenyl)-1, 4-pentadiene-3-one; 1, 5-bis (4-hydroxy-3-methoxyphenyl)-Penta-(1*E*, 4E)-1, 4-dien-3-one; 4"-(4"'-hydroxyphenyl-3-methoxy)-2"-oxo-3"-butenyl-3-(4'-hydroxyphenyl)- propenoate; Epiprocurcumenol; Isoprocurcumenol; Zedoaronediol; Procurcumenol; Curcumin L; Hopenone I; Gitoxigenin and 20-oxopregn-16-en-12-yl acetate) are proposed as the novel inhibitors against the SARS-CoV-2 main protease. Here, we demonstrated that using SwissADME online server tools that had all sixteen molecules has better "drug-likeness" than control and does not violate any Lipinski, Ghose, Veber, Egan or Muegge rules. As a 'BOILEDegg evaluation', predicts that all compounds except one has higher gastrointestinal absorption (HIA) than control chloroquine and is not effluxed by P-glycoprotein. Additionally, all the sixteen compounds does not penetrate the BBB and is not a substrate of the most Cytochrome P450 enzymes. Importantly, all sixteen compounds are more potent than chloroquine in treatment of against COVID-19 Mpro according to by using through *in silico* approach.

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