



Covid-19 prevention by blocking 6M3M from SARS CoV-2 of using *Allium sativum* extract: An in silico analysis

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Abstract

An infectious disease COVID-19 also known as “Corona virus disease 2019” which is caused by severe acute respiratory syndrome corona virus 2 (SARS-CoV-2). This global epidemic has been affecting millions of people within a short period of Time. Epidemic researchers are putting lot of efforts to discover a preventive traditional vaccine. The main objective of this article is to identify the phytochemicals as ligands which has the capability to deactivate the nucleo-capsid protein from SARS CoV-2(6M3M) that help for the growth of the virus. Molecular docking of phytochemicals with the viral proteins can be studied by the Biovia Discovery studio. The interaction of molecule was determined by the energy of -CDocker and-CDocker interaction respectively. More is the negative energy means high positive scores of these two parameters indicates that Caffeic acid can effectively inhibit the viral metabolic activity than other phytochemicals present in *Allium*. It can be predicted that these molecules can interfere with the infection phase of SARS-CoV-2 virus.

Keywords: *Allium*, phytochemicals, covid-19, biovia, SARS-CoV-2

Introduction

Globally, COVID-19 is considered as an infectious communicable serious pandemic disease. It is imparting life risk consequences for aged people in various countries. On 30th January, 2020 The World Health Organization (WHO) has declared that coronavirus outbreak is a Public Health Emergency of International Concern [1, 2] This epidemic were first preliminary reported at Wuhan city of China in December 2019 and gradually spread its tentacles worldwide [3, 4]. According to WHO a confirmatory case is that “if a person has undergone with laboratory confirmation of COVID-19 infection” [5]. Unfortunately till today no vaccine and preventive molecular drugs has developed to fight against this disease [6].

Nature has been a source of many medicines in the form of chemicals, enzymes and proteins present in the plants through which modern drugs have been derived [7]. The chemical substances produce by plant has some medicinal that can regulate or affect the human physiology are called as phytochemicals. These chemicals can be used as therapeutic purposes and these phytochemicals can extract from seed, barks, leaves, fruits and flowers etc [8]. These phytochemicals are have various medicinal properties like anti-oxidant, anti-diabetic, anti-cancer and anti-inflammatory. These molecules can serve as the initiators of production of pharmaceuticals which are Safe and cost effective [9].

About 25% of pharmaceutical drugs available in the market are of botanical origin and the beneficial effects are evaluated by invitro bioassay or experiments using animal models [10].

Garlic (*Allium sativum* L.) is a valuable spice and a popular remedy for various ailments and physiological disorders. Garlic oils are used in case hypercholesterolemia also reduces the systolic blood pressure.

Allium sativum belonging to family *Amaryllidaceae* is known to cure many fungal, viral, bacterial and parasitic infection. It is one of the earliest known medicinal plant which is used for health benefits that has sulphur containing compounds in the form of phytochemicals. The main objective of this study to identify phytochemicals present in *Allium sativum* to cure the corona virus disease COVID-19 by inhibiting its metabolism.

Materials and Methods

Biovia software (Dassault Systems of France) having Discovery Studio tool was analysed the molecular level interaction between the phytochemicals and enzymes. This software helps in prediction of molecular interaction through machine learning.

Plant produces phytochemicals as secondary metabolites to protect them from predators and plants usually fights against the microorganisms. The plant is known to contain phytochemicals like Caffeic acid, Ferulic acid, Coumaric acid, sinapic acid and Vanilic acid etc. The nucleo capsid protein from SARS CoV-2 (PDB: - 6M3M) is an important protein play a very crucial for the survival and multiplication of this virus.

Molecular interaction between the viral protein and phytochemicals which form a covalent bond to inhibit viral growth. Biovia discovery studio was used for analyzing the molecular interaction to identify the phytochemicals. Phytochemicals were selected from the plant and sdf file downloaded from the website. And PDB code of protein was downloaded from RCSB website. Active site as receptor cavity of this enzyme was selected as “receptor cavity” protocol found under tool “receptor-ligand interaction”. For C-Docking in Biovia Discovery studio, enzyme molecule was treated as the receptor molecule and the phytochemical was treated as the ligand. Both “-CDOCKER_ENERGY” and “-

CDOCKER_INTERACTION_ENERGY” were determined the strength of molecular docking. High C-Docker score considered as the efficient interaction between the phytochemicals and the viral enzyme. Therefore, high positive values predict the effect of phytochemicals on treatment of COVID-19.

Results and Discussion

Active site of the 6M3M play a major role during this insilico analysis. And it is an insilico-based molecular docking method and optimized for accuracy. -CDOCKER energy was calculated based on the internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction signifies the energy of the nonbonded interaction that exists between the protein and the ligand. The criteria for best interaction was chosen based on a) high positive

value of -CDOCKER energy and b) small difference between -CDOCKER energy and -CDOCKER interaction energy. Nucleo capsid protein and Caffeic acid interaction value is represented in Table-1 and has the highest positive score of -CDOCKER energy 21.2264kcal/mole and small value of the difference 0.6316 kcal/mole between - C DOCKER interaction energy and - C DOCKER energy. Thus, the results indicated that Caffeic acid can effectively deactivate 6M3M thereby interrupting the hydrolase activity which process the amino-terminal end of the replicase polyprotein to generate two or three replicase products of the virus. Higher positive values for Caffeic acid indicated that it was the most active ingredient against SARS-CoV virus. Thus, the key phytochemicals caffeic acid preventing COVID-19 caused by SARS-CoV2 virus,

Table 1: C-Docker results of phytochemicals of *Allium sativum* with 6M3M protein

Sl No	Phytochemicals	- C Docker energy	- C Docker interaction energy	Difference between - C Docker interaction energy and - C Docker energy	Remark
1	Caffeic acid	20.5948	21.2264	0.6316	Shows more interaction
2	Ferulic acid	12.1545	19.7401	7.5856	
3	Coumaric acid	17.1985	18.5634	1.3649	
4	Sinapic acid	14.4929	21.4553	6.9624	

Conclusions

From this it is concluded that *Allium sativum* has anti-viral properties against COVID-19. It is found that caffeic acid of *Allium sativum*, which can have an interaction with the viral protein nucleo-capsid significantly to prevent COVID-19. From the molecular docking analysis, it is found that caffeic acid can effectively interact with viral protein to deactivate the viral function. Other phytochemicals do not much influence on viral protein molecule to stop their life cycle. Therefore, it can be concluded caffeic acid present in *Allium sativum* has the medicinal values which will be help for curing COVID-19.

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