Biointerface Research in Applied Chemistry
Platinum Open Access Journal (ISSN: 2069-5837)

Article
Volume 11, Issue 1, 2021, 7981 - 7993
https://doi.org/10.33263/BRIAC111.79817993

Screening of Potent Inhibitors Against 2019 Novel Coronavirus (Covid-19) from *Alliumsativum and Allium cepa: An In Silico Approach*

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Received: 3.06.2020; Revised: 26.06.2020; Accepted: 28.06.2020; Published: 4.07.2020

Abstract: The infection of the global COVID-19 pandemic and the absence of any possible treatment options warrants the use of all available resources to find effective drugs against this scourge. Various ongoing researches have been searching for the new drug candidate against COVID-19 infection. The research objective is based on the molecular docking study of inhibition of the main protease of COVID-19 by natural compounds found in *Allium sativum* and *Allium cepa*. Lipinski rule of five and Autodock 4.2 was used by using the Lamarckian Genetic Algorithm to perform Molecular docking to analyze the probability of docking. Further, ADME analysis was also performed by using SwissADME, which is freely available on the web. In the present study, we identified S-Allylcysteine sulfoxide (Alliin), S-Propyl cysteine, S-Allylcysteine, S-Ethylcysteine, S-Allylmercaptocysteine, S-Methylcysteine, S-propyl L-cysteine with binding energies (-5.24, -4.49, -4.99, -4.91, -4.79, -4.76, -5.0 kcal/mol) as potential inhibitor candidates for COVID-19. Out of 7 selected compounds, alliin showed the best binding efficacy with target protein 6LU7. *In silico* ADME analysis revealed that these compounds are expected to have a standard drug-like property as well. Our findings propose that natural compounds from garlic and onion can be used as potent inhibitors against the main protease of COVID-19, which could be helpful in combating the COVID-19 pandemic.

Keywords: COVID-19; Garlic; Onion; 6 LU7; Molecular Docking.

1. Introduction

According to the situation report from the World Health Organization (WHO), more than 5,09,164 cases of coronavirus disease 2019 (COVID-19) have been reported worldwide till March 27, 2020. The new strain of COVID-19 was identified at the end of 2019, initially named 2019-nCoV, and emerged during an outbreak in Wuhan, China [1]. The Emergency Committee of the World Health Organization (WHO) declared an outbreak in China on January 30, 2020, which was considered to be a Public Health Emergencies of International Concern (PHEIC) [2, 3]. The pathogen caused the disease was soon identified as a novel coronavirus,

which belongs to the genus Beta coronavirus and is closely related to severe acute respiratory syndrome coronavirus (SARS-CoV) with 89.1% nucleotide similarity in the viral genome [4].

Later this was named as severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) by the International Committee on the Taxonomy of Viruses. Wang et al. from Wuhan Institute of Virology screened some of the FDA approved anti-viral or anti-infection drugs and found that remdesivir and chloroquine could effectively inhibit the virus in cell-based assay with EC50 of 0.77 and 1.13 μM, respectively [5]. Recently various clinical trials are ongoing for the treatment of COVID-19. However, there is currently no therapy available for the treatment of COVID-19. The therapies have been focused on targeting protease, helicase, polymerase, and using immunomodulators such as interferons and corticosteroids. Repositioning of drugs for use as anti-viral treatments is a critical need [6].

Bioinformatics is considered as one of the most important and innovative approaches in the design of new drugs. Various bioinformatics techniques are present, which would easily help in reducing the time of the experiment, possibility of error, high cost of clinical and laboratory trials. In Bioinformatics Molecular docking, target point determination and chemical stability studies are the most important methods used in drug design. One of the novel therapeutic strategies used for inhibition of virus infection is searching for an inhibitor of the enzyme in natural compounds as they have minimal side effects. Among natural compounds, our study was focussed on *Allium cepa* (Onion) and *Allium sativum* (Garlic).

Phytochemicals present in garlic and onion have been observed to block the formation of protein and genetic material in the virus [7-9]. Garlic possesses high anti-viral properties. For example, experiments have proved that garlic extract can minimize influenza A and B viral infections [10]. Similarly, garlic is effective against different viruses such as cytomegalovirus, rhinovirus, HIV, herpes simplex virus 1, herpes simplex virus 2, viral pneumonia, and rotavirus. In another study, garlic was observed to significantly minimize the occurrence of the common cold virus [11]. Organosulfur compounds like allicin, diallyl trisulfide, and ajoene are the main chemicals thatimpart anti-viral properties to garlic [12, 13]. It was observed that these chemicals affected the oxidative stress response mechanism [14]. Onion extracts were effective in decreasing infection of the New Castle Disease virus by blocking the attachment of the virus with the cell [15]. Onion and garlic are, therefore, important plants which could be used as an alternative treatment for viral infection and for the prevention of severe disease development [16].

In the continuation of ongoing research, our present study is designed to find effective natural therapeutic agents from garlic and onion that could show better inhibitory efficacy against the main protease of COVID-19 by using the molecular docking approach. The results of this study will provide better opportunities to other investigators with new ways to recognize and development of new COVID-19 treatment.

2. Materials and Methods

2.1. Requirements for In-silico analysis.

- Windows 10
- MGL tools
- Discovery Studio Visualizer
- Autodock 4.2
- Cygwin

- Binary files

2.2. Target used in docking.

The target used for docking is the major protease of the novel coronavirus (COVID-19). Its 3D structure is obtained from PDB (Protein Data Bank) (www.rcsb.org) having PDB ID: 6LU7 (Figure 1) in .pdb format. During the analysis, the water molecules were removed, and its energy was also minimized.

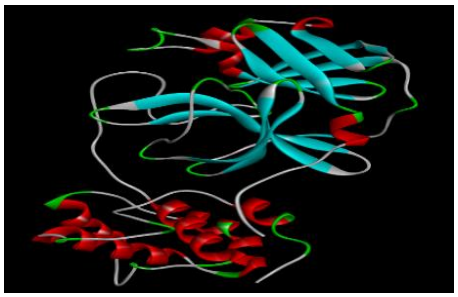


Figure 1. 3D structure of COVID-19(PDB ID: 6LU7).

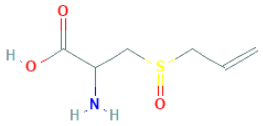
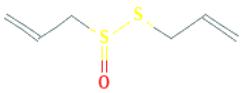
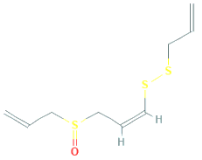
2.3. Ligand preparation.

Organosulfur compounds from*Allium sativum* (Garlic) and *Allium cepa* (Onion) were chosen for docking. Their 3D structure was obtained from PubChem in .sdf format. (https://pubchem.ncbi.nlm.nih.gov/).

2.4. Lipinski's rule of five.

All the 23 compounds were assessed for their oral bioavailability and drug-likeliness properties by Lipinski's rule of five. The natural compounds of garlic and onion are chosen for docking are mentioned below with their chemical structures and PubChem ID (Table 1 and 2).These entire sets on initial screening have a probable impact on the pharmacokinetics efficacy of drugs.

Table 1. Organosulfur compounds of *Allium sativum.*

S.No	PubChem_ID	Compound name	Chemical Structure
1	121922	S-Allylcysteine sulfoxide (Alliin)	
2	16590	Diallyl disulfide DADS	
3	65036	Diallyl disulfide-oxide (Allicin)	
4	11617	Diallyl sulfide DAS	
5	16315	Diallyl trisulfide	
6	66282	Allyl methylsulfide	
7	9881148	Z-Ajoene	

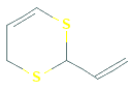
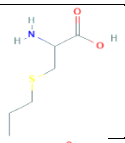
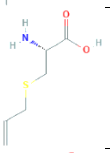
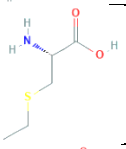
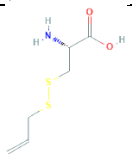
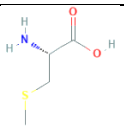
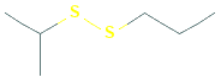
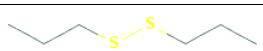
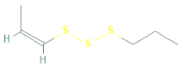
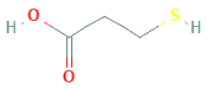
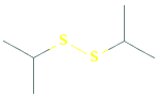
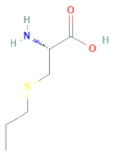
8	133337	2-Vinyl-4H-1,3-dithiine	
9	125198	S-Propyl cysteine	
10	9793905	S-Allylcysteine	
11	92185	S-Ethylcysteine	
12	9794159	S-Allylmercaptocysteine	
13	24417	S-Methylcysteine	

Table 2. Compounds of *Allium cepa.*

S.No	PubChem_ID	Compound name	Chemical Structure
1	16592	Methyl propyl disulphide	
2	118529	Isopropyl propyl disulphide	
3	19310	Dimethyl trisulphide	
4	12377	Dipropyldisulphide	
5	16591	2-Propenyl propyl disulphide	
6	12232	Dimethyl disulphide	
7	5352694	Cis-propenyl propyl trisulphide	
8	6514	3-mercaptopropionic acid	
9	77932	Bis(1-methylethyl) disulphide	
10	101975	S-propyl L-cysteine	

2.5. Docking Procedure.

Target-Ligand docking was performed in Auto dock 4.2 program Auto dock tools were used to get the best conformation of the target-ligand interaction. Scoring of target-ligand interaction was done on the basis of free energy of binding.The Lamarckian genetic algorithm (LGA) was applied to find the interaction pattern between the COVID-19 molecule and the

natural compounds of garlic and onion. A grid of 60, 60, and 60 points in the x, y, and z directions wereused on COVID-19 and the natural compounds of garlic and onion. In all docking procedures, 10 independent genetic algorithms were run with a population size of 150 for each molecule under studyLGA run was stopped after a maximum number of 2500000 energy evaluations and 27,000 maximum generations. The auto dock was then executed to obtain Docking Log Files (DLG) for further analysis.

2.6. ADME property characterization.

The physicochemical properties and the ADME parameters of the 7 compounds from *Allium sativum* and *Allium cepa* that showed best results were analyzed by web-based tool SWISSADME (http://www.swissadme.ch).

3. Results and Discussion

3.1. Lipinski's rule of five.

The drug-likeness properties such as molecular weight of the compound (MW), number of hydrogen bond donor (HBD) and acceptor (HBA) and calculated LogP (cLogP), of Allium sativum and Allium cepa compounds, were firstly evaluated by Lipinski's rule of five. Results showed that all the selected compounds follow Lipinski's rule of five. Table 3 and 4 represents the drug-likeness properties of Allium sativum and Allium cepa compounds analyzed by Lipinski's rule of five.

Table 3. Physicochemical properties of ligands of garlic accepting the Lipinski's rule of five.

S.No	PubChem_ID	Compound name	MW (≤500 daltons)	HBD (≤5)	HBA (≤10)	MolLog P (≤5)
1	121922	S-Allylcysteine sulfoxide (Alliin)	177.22	2	4	-1.33
2	16590	Diallyl disulfide DADS	146.27	0	0	2.39
3	65036	Diallyl disulfide-oxide (Allicin)	167.27	0	1	1.59
4	11617	Diallyl sulfide DAS	114.21	0	0	2.14
5	16315	Diallyl trisulfide	178.34	0	0	2.68
6	66282	Allyl methylsulfide	88.17	0	0	1.53
7	9881148	Z-Ajoene	234.40	0	1	2.52
8	133337	2-Vinyl-4H-1,3-dithiine	14.26	0	0	2.21
9	125198	S-Propyl cysteine	163.24	2	3	-0.33
10	9793905	S-Allylcysteine	161.22	2	3	-0.45
11	92185	S-Ethylcysteine	149.21	2	3	-0.73
12	9794159	S-Allylmercaptocysteine	193.29	2	3	-0.22
13	24417	S-Methylcysteine	135.18	2	3	-1.06

Table 4. Physicochemical properties of ligands of *Allium cepa* accepting the Lipinski's rule of five.

S.No	PubChem_ID	Compound name	MW (≤500 daltons)	HBD (≤5)	HBA (≤10)	MolLog P (≤5)
1	16592	Methyl propyl disulphide	122.25	0	0	1.92
2	118529	Isopropyl propyl disulphide	150.31	0	0	2.60
3	19310	Dimethyl trisulphide	126.26	0	0	1.51
4	12377	Dipropyldisulphide	150.31	0	0	2.66
5	16591	2-Propenyl propyl disulphide	148.29	0	0	2.52
6	12232	Dimethyl disulphide	94.2	0	0	1.34
7	5352694	Cis-propenyl propyl trisulphide	180.35	0	0	2.86

S.No	PubChem_ID	Compound name	MW (≤500 daltons)	HBD (≤5)	HBA (≤10)	MolLog P (≤5)
8	6514	3-mercaptopropionic acid	106.14	1	2	0.36
9	77932	Bis(1-methylethyl) disulphide	150.31	0	0	2.54
10	101975	S-propyl L-cysteine	163.24	2	3	-0.33

3.2. Molecular docking simulations.

Molecular docking studies were performed by using AutoDock tool 4.2. The binding energies of the garlic and onion compounds were illustrated in Tables 5 and 6.

Table 5. Docking results of COVID-19 (PDB_ID: 6LU7) with different ligands of garlic.

S. No.	Ligand	PubChem_ ID	Autodock				
			Binding Energy (kcal/mol)	No. of H-bonds	Total Internal Energy	Estimated inhibition constant, Ki	Residues
1	S-Allylcysteine sulfoxide (Alliin)	121922	-5.24	2	-1.6	143.76	Target:A: GLU290:OE1 Target:A: LYS5:HZ2
2	Diallyl disulfide DADS	16590	-2.44	0	-0.09	16.25	----
3	Diallyl disulfide-oxide (Allicin)	65036	-3.36	1	-0.22	3.43	Target:A:GLN110:HE21
4	Diallyl sulfide DAS	11617	-2.54	0	-0.11	13.64	----
5	Diallyl trisulfide	16315	-2.06	1	-0.14	32.73	Target:A:GLN127:O
6	Allyl methylsulfide	66282	-2.14	0	-0.03	26.79	----
7	Z-Ajoene	9881148	-2.94	1	-0.26	6.96	Target:A:SER158:HG
8	2-Vinyl-4H-1,3-dithiine	133337	-3.34	1	-0.04	3.54	Target:A:ASN151:OD1
9	S-Propyl cysteine	125198	-4.49	4	-1.51	514.26	Target:A:GLN127:O Target:A: LYS5:HZ2 Target:A: GLU290:OE1 Target:A: LYS5:HZ3
10	S-Allylcysteine	9793905	-4.99	2	-1.37	218.37	Target:A: ASP295:OD1 Target:A:THR111:HN
11	S-Ethylcysteine	92185	-4.91	3	-1.34	251.97	Target:A: GLU290:OE1 Target:A: LYS5:HZ2 Target:A: GLN127:O
12	S-Allylmercaptocysteine	9794159	-4.79	1	-1.57	310.08	Target:A: GLU290:OE1
13	S-Methylcysteine	24417	-4.76	4	-1.66	324.24	Target:A:THR111:HN Target:A:THR111:OG1 Target:A:GLN110:HE21 Target:A:ASN151:OD1

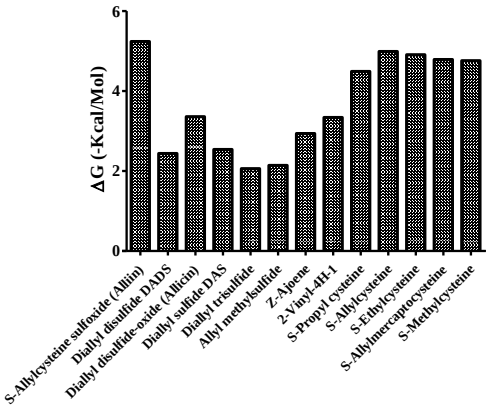


Figure 2. Molecular docking results between 6LU7 and drug candidate compounds of *Allium sativum* (the binding energy value ΔG is shown in minus kcal/mol).

The docking results exhibited that 7 natural compounds showed best binding energies with target protein 6LU7 viz, S-Allylcysteine sulfoxide (Alliin), S-propyl L-cysteine, S-Allylcysteine, S-Ethylcysteine, S-Allylmercaptocysteine S-Methylcysteine, and S-Propyl cysteine, and binding energy is -5.24, -5, -4.99, -4.91, -4.79, -4.76 –and 4.49 Kcal/mol, respectively (Fig. 2 and 3).

Table 6. Docking results of COVID-19 (PDB_ID: 6LU7) with different ligands of *Allium cepa*.

S.No	Ligand	PubChem_ID	Autodock				
			Binding Energy (kcal/mol)	No. of H-bonds	Total Internal Energy	Estimated inhibition constant, Ki	Residues
1	16592	Methyl propyl disulphide	-2.31	0	-0.02	20.12	-----
2	118529	Isopropyl propyl disulphide	-3.02	0	-0.09	6.15	-----
3	19310	Dimethyl trisulphide	-2.21	0	0	23.81	-----
4	12377	Dipropyldisulphide	-2.66	0	-0.16	11.26	-----
5	16591	2-Propenyl propyl disulphide	-2.61	0	-0.14	12.28	-----
6	12232	Dimethyl disulphide	-1.99	0	0	34.66	-----
7	5352694	Cis-propenyl propyl trisulphide	-3.19	0	-0.17	4.63	-----
8	6514	3-mercaptopropionic acid	-2.51	2	0.02	14.35	Target:A:GLU290:OE1 Target:A:LYS5:HZ2
9	77932	Bis(1-methylethyl) disulphide	-3.3	0	-0.08	3.83	3.83
10	101975	S-propyl L-cysteine	-5	1	-1.4	218.04	Target:A:LYS5:HZ2

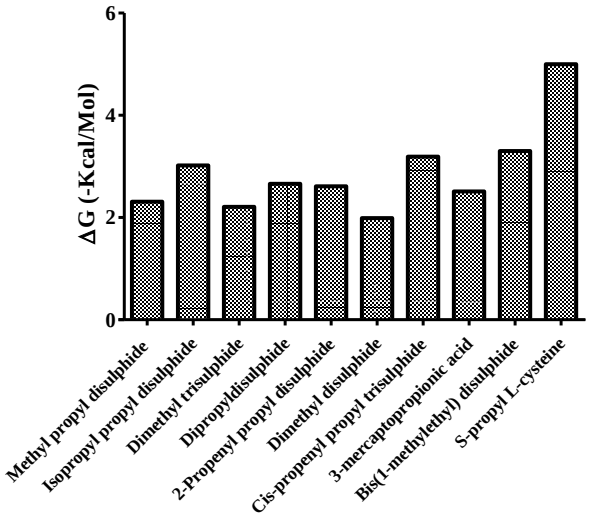
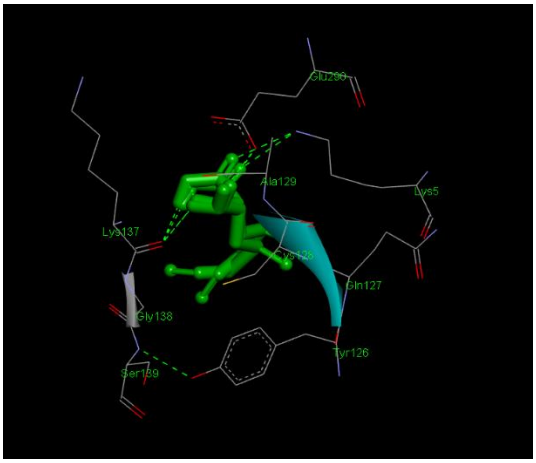


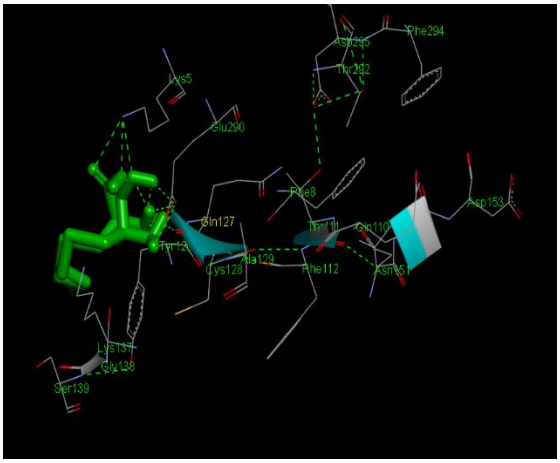
Figure 3. Molecular docking results between 6LU7 and drug candidate compounds of *Allium cepa* (the binding energy value ΔG is shown in minus kcal/mol).

The binding efficacy of the ligands within the active site of target protein main protease was further studied by using the Discovery studio visualizer, which provides a visualization of the ligand-protein interaction. The binding interactions of the alliin with target protein 6LU7

showed binding via two hydrogen bonds at GLU290:OE1 and LYS5:HZ2 amino acid residues (Fig. 4A). The binding site of S-propyl L-cysteine was observed to form a hydrogen bond at LYS5 residue (Fig. 5). For S-allylcysteine, binding sites were ASP295:OD1 and THR111:HN (Fig. 4C).



(A) S-Allylcysteine sulfoxide (Alliin)



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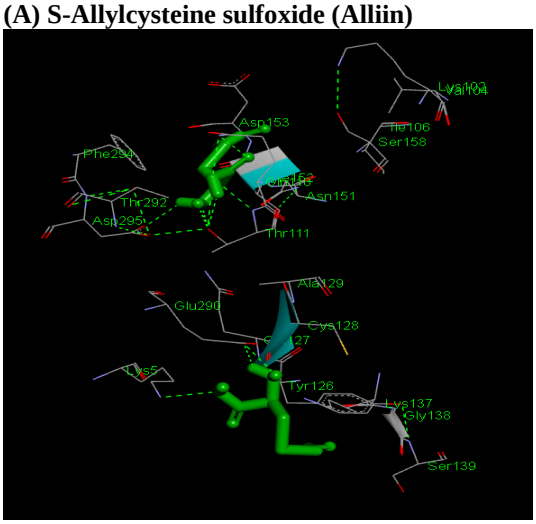
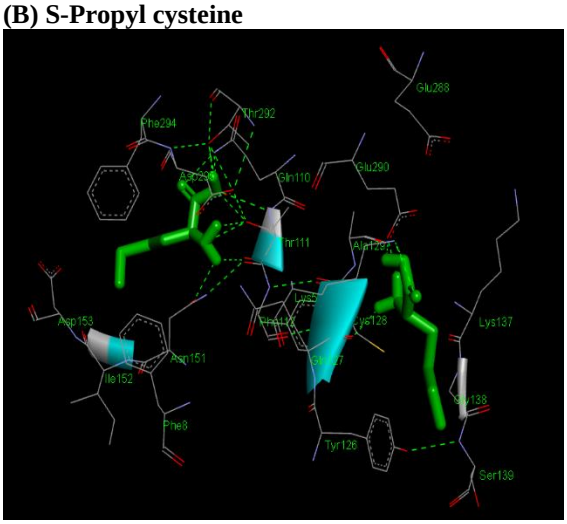
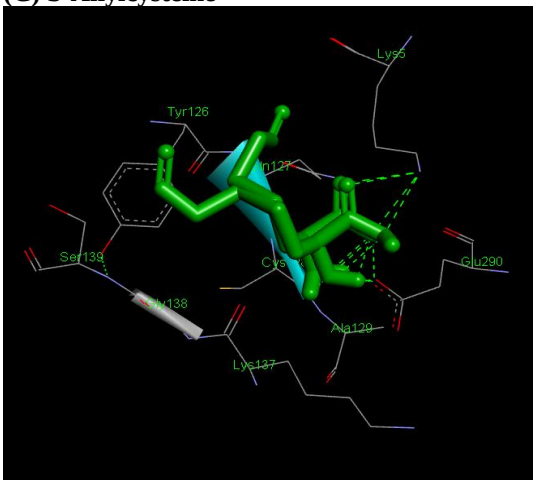


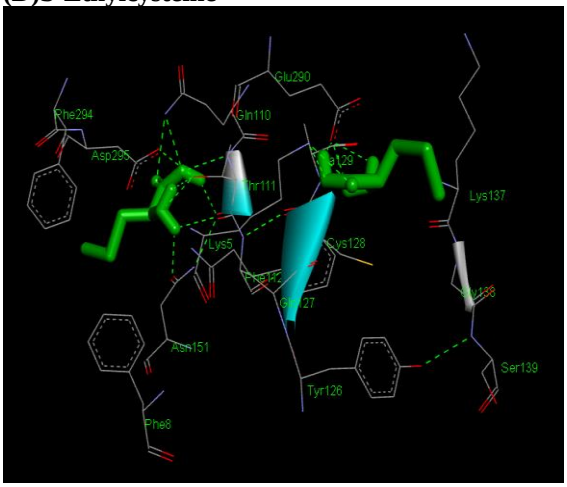
(C) S-Allylcysteine



(D)S-Ethylcysteine



(E) S-Allylmercaptocysteine



(F) S-Methylcysteine

Figure 4. Docking analysis visualization of 6LU7 binding with *Allium sativum* (garlic) compounds thathave shown better result (Binding Energy) than Hydroxychloroquine (Green dash lines show Hydrogen binding).

For S-Ethylcysteine, S-Allylmercaptocysteine, S-Methylcysteine and S-Propyl cysteine the amino acids associated were GLU290:OE1, LYS5:HZ2 and GLN127:O (Fig. 4D);

GLU290:OE1 (Fig. 4E); THR111:HN and THR111:OG1 (Fig. 4F) and GLN127:O, LYS5:HZ2, GLU290:OE1 and LYS5:HZ3 (Fig. 5) respectively.

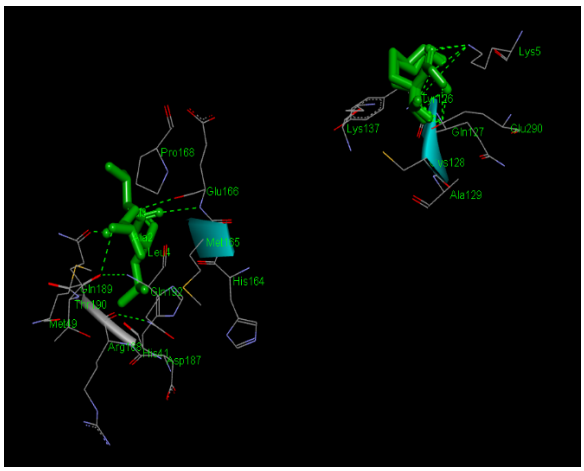


Figure 5. Docking analysis visualization of 6LU7 binding with S-Propyl L-cysteine *Of Allium cepa*, which has shown better results (Binding Energy) than Hydroxychloroquine (Green dash lines show Hydrogen binding).

The amino acid residues are responsible for the hydrophilic and hydrophobic interactions, which were considered as an important player in the binding of these types of inhibitors inside the active site of target protein 6LU7. Out of these 7 compounds, alliin showed better binding efficacy in terms of lower binding energy with a target protein. In addition to these, we have also compared our results with proposed drug hydroxychloroquine and found that alliin showed better molecular properties in comparison to this drug. The binding energy of hydroxychloroquine was found to be -3.61 Kcal/mol (Table 7, Fig. 6).

Thus, based onthe results of *in silico* study, alliin showed the best efficacy against selected target protein of COVID-19 and thus could be used as the potential therapeutic agent for COVID-19 treatment.

Table 7. Docking results of COVID-19 (PDB_ID: 6LU7) with proposed drug, hydroxychloroquine.

S. No	Ligand	PubChem_ID	Autodock				
			Binding Energy (kcal/mol)	No. of H-bonds	Total Internal Energy	Estimated inhibition constant, Ki	Residues
1	Hydroxychloroquine	3652	-3.61	0	-0.22	2.27	-----

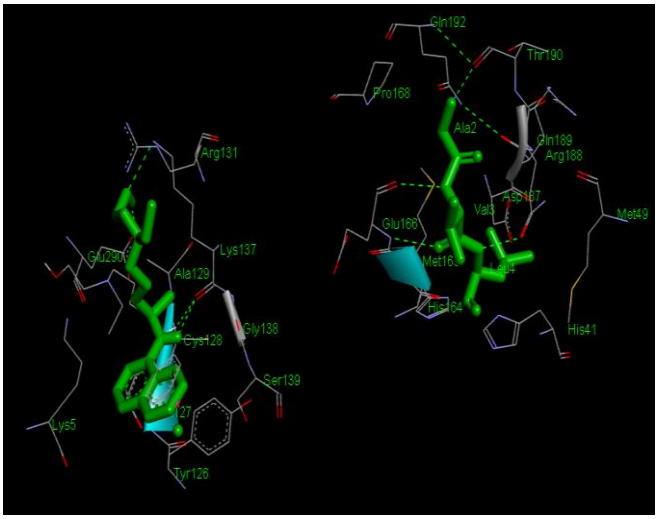


Figure 6. Docking analysis visualization of 6LU7 binding with Hydroxychloroquine (Green dash lines show Hydrogen binding).

3.3. Toxicity prediction by ADMET analysis.

The drug-like properties of the selected compounds, which showed better scores during docking analysis arealso estimated via ADME analysis. ADME analysis can be used to target key optimization attempts to augment the desirable features of a target compound. The ADME prediction analyzed by SWISSADME for the best 7 compounds isshown in Figure 7. Our results clearly showed that more or less all the predicted properties of the compounds were in the range, as revealed by SwissADME of standard oral drugs.

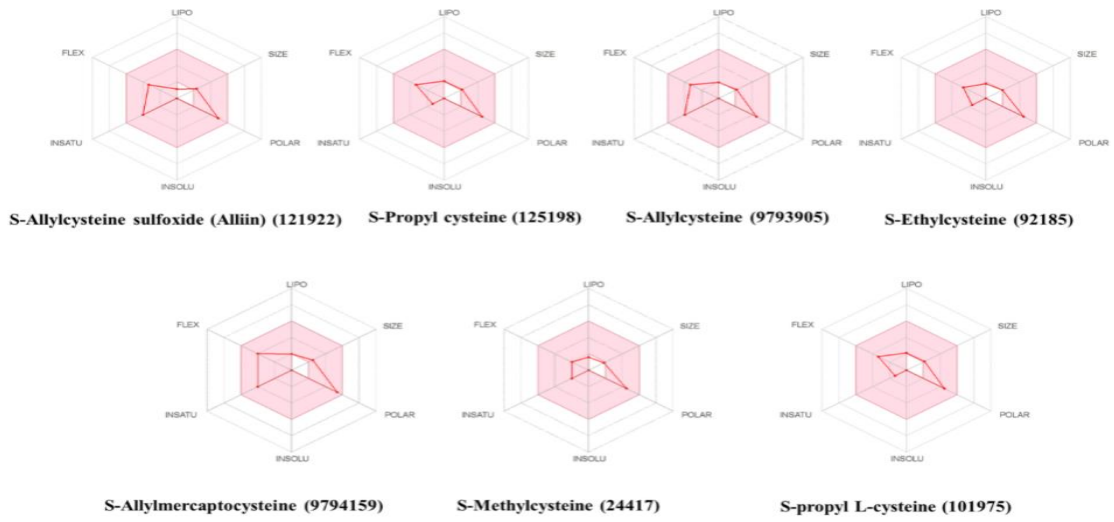


Figure 7. ADME parameters of compounds thathave shown better efficacy than hydroxychloroquine. The colored zone is asuitable physicochemical space for oral bioavailability. LIPO (Lipophility): -0.7 <XLOGP3< +5.0. SIZE: 150 g/mol<TPSA< 130Å2. INSOLU (Insolubility): 0<LogS (ESOL) < fraction Csp3 < Number of rotatable bonds <9.

3.4. Discussion.

COVID-19, which was emerged in China, has been affected now all world and become a major threat worldwide. It belongs to a class of viruses thatcan cause an infection inside humans and most of the vertebrate animals.This virus can affect the human liver, digestive, respiratory, and central nervous systems [17]. Viral main protease plays a pivotal role in coronavirusreplication. This enzyme is responsible for the cleavage of the polyprotein, producing functional proteins that will be packed into the virion [18].

In several viruses, proteases are responsible for viral replication and produce functional protein after proteolytic cleavage. Thus, proteases are considered as potent and suitable protein targets for the development and improvement of anti-viral based drug therapies [19]. This study aimed towards the main protease (M^{Pro}) i.e. chymotrypsin-like protease ($3CL^{pro}$) of COVID-19 as therapeutic target. This protease has been successfully structured and repositioned in PDB (PDB ID: 6LU7) and considered as a possible target protein to inhibit the infection of the virus by inhibiting its replication. The discovery and sequencing of the COVID19 protease structure (M^{Pro}) provide a possibility to screen potential drug therapeutics for the treatment and controlling its outbreak.

However, still no drugs are approved for the treatment of this disease. Thus currently, there is an urgent need for therapeutic alternatives. In order to add some more positive attribute to ongoing research related with screening and development of more significant drugs, the present study we evaluated interactions between viral protease (MPro) and natural compounds

of garlic (*Allium sativum*) and onion (*Allium cepa*) and also compare them with drugs in use for the treatment of COVID-19 like hydroxychloroquine. In order to identify the best suitable compounds against the COVID-19 infection pathway, compounds were selected on the basis of binding energies via the molecular docking approach.

As introduced earlier, it is already known that garlic and onion possess anti-viral properties, so based on that, here we established an *in silico* approach for the establishment of inhibition potential of 23 compounds of garlic and onion (Table 1 and 2).

In the present study, the different drug-likeness parameters like molecular weight, hydrogen bond donor, acceptor, etc., were calculated by Lipinski's rule of five were calculated. Lipinski's rule of five is a standard criterion to assess drug likeliness of a particular chemical compound having certain pharmacological properties that would help in making it a possible drug candidate in humans. These predictions have significant contributionsin the final result as well as further in silico analysis, thus savingthe time and economically more sustainable. Our results showed that selected compounds of *Allium sativum* and *Allium cepa* are in accordance with the drug-likeness properties of Lipinski's rule of five (Table 3 and 4).

Results from the previous study have also used Lipinski's rule of five for a screening of anticancer compounds from natural resources [20].

Molecular docking analysis was implemented with these 23 compounds against target protein 6LU7 of COVID-19. Molecular docking is an *in silico* based approach that focused on the identification of non-covalent interactions between receptor protein and ligand molecules. This computational tool analyzes the mode of receptor-ligand interaction for an established binding site, and affinity or strength of a ligand-target protein association is evaluated by binding energy prediction. The selection of compounds, is done on the basis of lower binding energy against specific target receptor protein and considered as a probable drug for a particular disease. Molecular docking analysis of major protease 6LU7 with 23 compounds of garlic and onion revealed that only 7 compounds (S-Allylcysteine sulfoxide (Alliin), S-propyl L-cysteine, S-Propyl cysteine, S-Allylcysteine, S-Ethylcysteine, S-Allylmercaptocysteine, S-Methylcysteine) the best-docked score in terms of binding energies and were found to be best compound against target protein (Fig. 2 and 3, Table 5 and 6).

Out of 7 best compounds, S-Allylcysteine sulfoxide (Alliin) has shown the lowest compound binding energy (-5.24 Kcal/mole) and two hydrogen bond interactions with GLU290 and LYS5 residues (Fig. 4 and 5). Furthermore, we have also compared our natural compounds with proposed drug molecule hydroxychloroquine and found that it shows lower binding efficacy in comparison to our best-selected compound alliin with a binding energy of -3.61 Kcal/mole (Fig. 6). Therefore, we suggested that alliin alone or in combination with a currently used therapeutic drug could be considered as a potential anti-viral agent with minimal side effects in the prevention of COVID-19. These findings are in support of previously reported studies thatsuggested the inhibitory role of natural compounds against major protease of COVID-19 via *in silico* based methods [17, 21-23].

Further, the drug likeliness of these compounds wasalso analyzed by ADME (Absorption, Distribution, Metabolism, and Excretion) parameter which helps to overcome the pharmacokinetics-related failure in clinical phases (Table. 3 and 4). These criteria govern the molecular characteristics which are essential for pharmacokinetics of drug inside the human body such as absorption, distribution, metabolism, and excretion (ADME) [24]. From the ADMET prediction, we observed that selected compounds, including alliin possess better drug-likeness properties as well as less toxic effects (Fig. 7). Thus it could be suitable for further

investigation and could be used as drug-like molecules against the target protein of COVID-19. Other anti-virals have been evaluated in SARS-CoV-2 as the polymerase inhibitor remdesivir, a nucleotide analog (currently in clinical trials against Ebola virus and SARSCoV-2), alone or in combination with chloroquine, an inhibitor of lysosome acidification, with interesting results [25]. However, these *in silico* based studies areonly one method of predicting the anti-viral potential of the compounds involved. Altogether, this study will immensely help in finding better therapeutic agents which inhibit viral replication by targeting the main protease of COVID-19 and add more attributes in ongoing research for the development of effective treatment options against COVID-19. Therefore, further in vitro and in vivo experimental studies required to confirm the anti-viral activity of these compounds against COVID-19 treatment.

4. Conclusions

In summary, our present study attempted to explore the potential of effective natural compounds from garlic and onion against the main protease of COVID-19 in comparison to proposed drug hydroxychloroquine. We have selected 23 effective compounds from these two plants and out of 23 compounds 7 compounds found as the most potent inhibitors against COVID-19 target protein 6LU7. Our results from molecular docking exhibit that alliinshowed the best binding efficacy against COVID-19 Main Proteases, which can further encourage us to examine its potential in pre-clinical and clinical studies.

Funding

This research received no external funding.

Acknowledgments

The authors thank the management of Noida Institute of Engineering & Technology and Lucknow University for providing the facilities to carry out this study.

Conflicts of Interest

The authors declare no conflict of interest.

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