In silico screening of phytochemicals from *Brassicaceae* family as potential antiviral drugs against Crimean-Congo hemorrhagic fever

Hamza Bacha*, Anwar Hussain*, Sufaid Khan*, Nizar Nawaz*, Majid Khan*

* Department of Botany, Abdul Wali Khan University Mardan

Abstract- Crimean Congo Hemorrhagic fever is a widespread disease caused by a tick-borne virus (Nairovirus) in the family Bunyaviridae. This disease has been reported in most parts of the Asian, African and the European countries and needs proper attention. During current study we carried out virtual screening of a library of different phytochemicals with Crimean Congo hemorrhagic fever virus OTU protease and another protein target using molecular docking approach. A total of 146 secondary metabolites reported from different plants were docked. The amino acids sequence of the given proteins as well as closely related species were obtained from NCBI and were then stored in FASTA format. Using MEGA6 software these sequences were aligned and the homology between these sequences was observed. The target proteins were docked with the database of phytochemical and results were interpreted. Interestingly four phytochemicals from the class Glucosinolates showed strong interactions with active sites of the target proteins with lowest binding energies. These phytochemicals were also docked with a similar human protein but fortunately no interaction was shown. Thus it is suggested that the phytochemicals mentioned above may be screened in vitro and in vivo to be further established as potential drugs against the CCHFV.

Index Terms- Congo virus; Glucosinolates; Docking; MEGA6

I. INTRODUCTION

Crimean-Congo hemorrhagic fever is a tick borne viral disease caused by virus which belongs to the family Bunyaviridae [1]. The ticks of genus Hyalomma particularly the *Hyalomma marginatum* is the primary vector of Crimean Congo hemorrhagic fever virus. Their ability of human to human spreading, the fear that it may be used as bioterrorism agent and the evidences that the disease is getting increases day by day make it an important human pathogen and a critical topic to work on.

A case reported from present Tajikistan in the 12 century might be the starting point and an initial event of Crimean-Congo hemorrhagic fever [2]. In the mid-20th century several cases were reported from Crimea region where more than 200 people died of this fatal disease. Soviet scientist for the first time predicted this sickness in 1944 [3]. They coined its name as Crimean Congo hemorrhagic fever but they were unable to isolate and inspect the causal agent i-e Crimean Congo hemorrhagic fever virus. CCHF is widespread in countries like Africa, the Balkans, the Middle East and Asian countries south of the 50th parallel north – the geographical limit of the principal tick vector.

Among these Iraq is one of the eastern Mediterranean countries where CCHF is endemic and spreading with a higher rate. The first victim of this virus in Iraq has reported since 1979 when the disease was first detected in ten patients. Since then, six major cases were reported in between 1989 and 2009; moreover a total of 11 cases has been reported in 2010; three deadly cases were reported in 2018; and more recently 33 confirmed cases including 13 deaths (CFR 39%) were reported in 2021. The health authorities of Iraq notified WHO about 212 cases of CCHF from 1 January to 22 May. Among these 212 cases, 115 (54%) were suspects and 97 (46%) were laboratory confirmed. The fatality rates among these cases were high i-e there were total 27 deaths reported among which 14 deaths were in suspected cases and 13 in laboratory confirmed cases. The number of CCHFV cases reported in the first five months of 2022 are considerably high i-e about 33 laboratory confirmed cases were recorded [4].

Similar to other viruses of this family, CCHF virus has a single stranded negative-sense RNA virus with a proper covering (envelope). The viral RNA is tripartite and can be documented as Small (S), the Medium (M) and the large (L) fragments according to their size [5]. The S fragment is the smallest fragment and encodes the important Nucleocapsid protenaceous component. Its major function is to guard the RNA and have role in viral transcription and replication. The M segment usually encodes the glycoproteins. The glycoproteins are the G1 and G2 glycoproteins. These glycoproteins projects through the viral lipid protein envelope and accounts for viral anchoring to the host cell [6]. The L-fragment encodes for viral RNA-dependent RNA polymerase which is involved in the RNA replication process. The L-fragment of Crimean Congo hemorrhagic fever virus has nearly two fold larger size than other members of family Bunyaviridae [7].

RNA-dependent RNA polymerase is the important proteins of Crimean Congo hemorrhagic fever virus encoded by its genetic machinery. OTU protease is responsible for catalyzing new RNA strand during the replication process. In the same way nucleoprotein is the second major protein of Crimean Congo

hemorrhagic fever virus having the property of DNA specific endonuclease activity in the present of metals.

As for as treatment of CCHF is concerned, there is no drug approved by the FDA, however supportive therapy of the patient is highly recommended. Even though there is no official drug approved, the antiviral drug ribavirin is considered beneficial during the course of sickness. A major problem in using the antiviral drug ribavirin is its synthetic nature due to which it has many side effects in which anemia is the highlighted one [8]. There is an urge to develop a drug which would be natural and life friendly. Therefore we are making an approach to screen the phytochemicals of *Brassica oleraceae* var. *italica* as potential antiviral drugs against CCHF.

In current study, In-silico approach in used for the identification of the novel drugs against the CCHF as this approach has been of great importance to develop fast, accurate and precise target identification and estimation methods for the discovery of drugs. The conventional methods of drug designing were based on trial and error, which were long, tidy and expensive methodologies. Moreover, once a drug is discovered, it must undergo preclinical and clinical tests and then it must get the FDA approval. Due to limitation of the cost and accuracy, experimental techniques cannot be applied widely. Therefore modern drug designing has shifted to in-silico approaches for the fast, precise and accurate discovery of drugs.

Medicinal plants are used all over the world for the treatment of many lethal diseases as they contain a diverse amount of useful phytochemicals. Broccoli species are known for processing many secondary metabolites have strong anti-oxidant and inhibitory activities [9]. Broccoli contains precursors of sulforaphane, the most active natural activator of Nrf2. Fermented vegetables comprise many lactobacilli, which are also effective Nrf2 activators. Nrf2 (Nuclear factor (erythroid-derived 2)-like 2) anti-oxidant transcription factor may be of primary importance. Nrf2 is the main regulator of the antioxidant response in humans. It modulates the expression of hundreds of genes, including not only the antioxidant enzymes (i-e, glutathione related), but also the large number of genes that control seemingly disparate physiopathological processes [10]. Due to inhibitory activities of various metabolites of broccoli, we have screened out some of its important phytochemicals as inhibitors against the OTU protease and Nucleoprotein of Crimean Congo hemorrhagic fever virus using techniques of the bioinformatics. The basic aim of this research is to find out phytochemicals which could serve as inhibitor against these proteins and hence could be used a drug against the brutal disease CCHF.

2. MATERIALS AND METHODS

2.1 Selection of a target proteins:

Literature was consulted in order to identify different domains and proteins that could be inhibited and then could result in better response of human immune system against the CCHFV. The Ovarian tumor (OTU protease) domain of CCHFV and the Nucleoprotein of CCHF were selected because of their importance in viral multiplication. The sequence of the OTU protease and Nucleoprotein were retrieved from the database of National Centre for Biotechnology Information (NCBI;-www.ncbi.nlm.nih.gov). The sequences were then stored in FASTA format on the local computer. The retrieved sequences were then subjected to BLASTn homology search in order to identify the homologous proteins from closely related virus including Dugbe virus, Hazara virus and Nairobi sheep disease virus. The sequences of the proteins of the given viruses were also stored in FASTA format.

The sequence of the target domain and protein was then aligned with the closely related proteins by using multiple sequence alignment program CLUSTALW implemented in Molecular Evolutionary Genetics Analysis (MEGA) software. The MEGA 6 software is designed for the homologous gene sequences from same species or from different species.

Crystal structures (3D) of OTU domain OTU protease and the Nucleoprotein were obtained from the Protein Databank with the help of PDB codes i-e 3PHU and 3U3i respectively. The crystal structures of OTU protease OTU protease and the Nucleoprotein were downloaded and saved in Brookhaven Protein Databank (PDB) file format.

Software (CHIMERA1.10.1 lnk) was used to remove the attached tags from the targeted domain by selecting the tags and pressing the Delete button leaving pure crystal OTU domain OTU protease. These tags are generally used to purify the recombinant proteins. However, the Nucleoprotein was available in its native form without any compounds or tags attached to it. These crystal proteins were saved in PDB format and were then used in MOE software (Molecular Operating Environment) for docking purpose.

2.2 In silico analysis of the phytochemical with targeted proteins (Docking):-

In order to find out a suitable phytochemical which could be used as a drug for CCHF, Broccoli plant was selected. Broccoli plant contains many important phytochemicals from the class glucosinolate. 3D structures of the selected phytochemicals including like Glucosinolates, Alkaloids, Benzoquinones, Coumarins, Flavanones, Flavones, Iso-flavones and Xanthones were prepared by using Chemdraw software(RRID:SCR_016768) and all the structures were then kept in the MDL Molfile format. Molecular operating environment (MOE) was used to prepare and store library of the selected phytochemicals [11]. The PDB structures of the target proteins were uploaded one by one to the MOE. Energy of these structures were minimized by selecting compute and protonate 3D. The energy minimized structure was then saved in PDB format. For carrying virtual screening of phytochemicals through molecular docking PDB structures of OTU protease & Nucleoprotein were opened in different tests in MOE. The active sites of these proteins were identified by selecting compute and then the site finder option. After the active sites of these proteins were selected, the compute option was again selected in which the Dock option leads us to a new window. Here the data base of the phytochemicals which was created earlier was uploaded to the ligand atoms, selecting London DG as rescoring 1 and rescoring 2. In the retain option of both rescoring 1 and 2 the 10 option was selected (for 10 poses) and then docking was started. After 30 to 40 minute the docking process completed and the results were stored in MOE format.

3. RESULTS

3.1. Protein homology

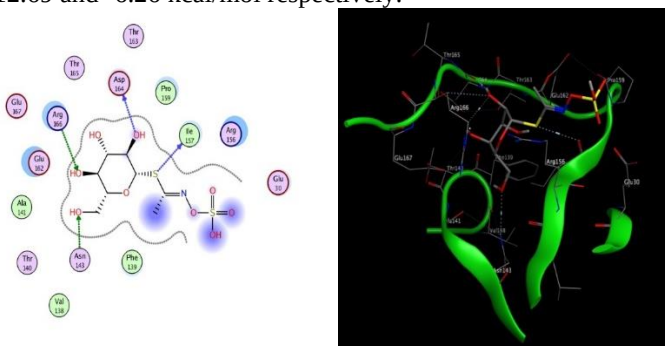
The sequences of RNA dependent RNA polymerase and Nucleoprotein of the Crimean Congo hemorrhagic fever virus were blasted with the nearest human pathogen like Dugbe virus, Hazara Virus and Nairobi Sheep disease virus. The retrieved sequences were then combined and aligned by the MEGA6 software in separate tests. The similarity shown by OTU protease with the proteins of the above listed viruses was about 18.37%. In the same way the homology shown by the Nucleoprotein of the Crimean Congo hemorrhagic fever virus with the proteins of the listed viruses was 41.71%. This give us a clear clue that the proteins of these virus have similarity in sequences and hence the screened phytochemical might inhibit these proteins too.

3.2. Molecular Docking of OTU protease and Nucleoprotein with the selected Phytochemicals

The binding cavity of OTU protease consists of 17 amino acids which include PHE29, LEU48, VAL138, PHE139 THR140, ALA141, VAL142, ASN143, LEU155, ARG156, ILE157, GLU162, THR163, ASP164, THR165, ARG166 and GLU167. Similarly active site of the Nucleoprotein consists of 74 amino acids thus making a large cavity. Amino acid present in the binding cavity of the Nucleoprotein are GLN58, LYS59, ASP60, SER61, TYR63, ALA64, SER65, LUE67, VAL68, THR71, VAL152, MET173, ARG176, ARG177, LEU179, ILE180, ALA296, LEU297, ALA299, GLN300, ALA302, GLN303, ILE304, THR306, LEU331, LEU334, GLY335, GLN337, PRO338, ARG339, GLY340, THR341, LYS342, LYS343, MET344, ARG372, ILE373, TYR374, MET375, HIS376, PRO377, THR381, ALA382, GLY383, ARG384, ILE385, SER386, GLU387, GLY389, GLY408, HIS409, THR410, LYS411, GLN437, PHE441, MET446, ASP447, ILE448, VAL449, ALA450, GLU452, HIS453, LEU454, HIS456, GLN457, VAL460, LYS462, ALA469, TYR470, VAL472, LYS473, GLY474, ASN475 and ALA476. When these active sites of the energy minimized structures of OTU protease and Nucleoprotein were docked with the listed phytochemicals, good interaction was shown by many phytochemicals. In this study, we have excluded those phytochemical ligands that violate Lipinski's rule of five[8]. That is, ligands with MW > 500 g/mol, hydrogen-bond-donating atoms > 5, hydrogen-bond-accepting atoms > 10, or Clog P > 5, even though they may have strong docking energies, were not considered. Four phytochemicals belonging to the class Glucosinolate showed strong interaction exactly with in these binding cavities. These phytochemicals include Glucocapparin, Gluconasturtiin, Glucobrassicin and Sinigrin with lowest binding energies and obeying the Lipinski's rule of five.

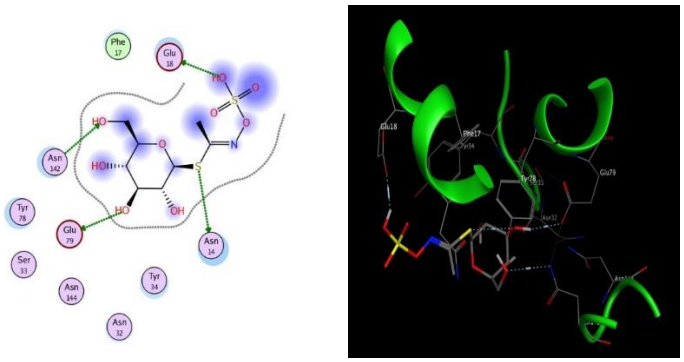
3.2.1. GLUCOCAPPARIN:-

Glucocapparin interact with the active sites of both the target proteins. Interaction has been with the OTU protease at the amino acid no, 143, 157, 164 and 166 (Figure 1). In the same way this phytochemicals interacts with the Nucleoprotein at the amino acid no, 14, 18, 79 and 142 (Figure 2). These phytochemicals obeys the Lipinski rule for drug likeliness (8). Binding energy of the phytochemical with both the proteins is -12.69 and -6.26 kcal/mol respectively.



(a) (b)

Figure 1. Interaction of the phytochemical Glucocapparin from broccoli with the OTU protease of Crimean Congo hemorrhagic fever virus. (**a) 2D** view of interaction between Glucocapparin with OTU protease of Crimean Congo hemorrhagic fever virus. Interaction has been made on the amino acid no, 143, 157, 164 and 166 respectively. The binding energy of the ligand during the docking process was -12.69kcal/mol; (**b**) **3D** view of interaction between Glucocapparin and the OTU protease of Crimean Congo hemorrhagic fever virus.

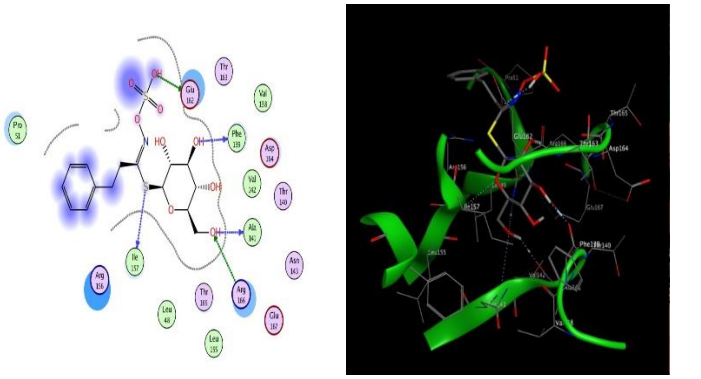


(a) (b)

Figure 2. Interaction of Glucocapparin from broccoli with the Nucleoprotein of Crimean Congo hemorrhagic fever virus. (**a) 2D** view of interaction between Glucocapparin and the Nucleoprotein of Crimean Congo hemorrhagic fever virus. Interaction has been made on the amino acid no, 14, 18, 79 and 142. Weight of the ligand was 333.34g/mol and the binding energy during the docking process was -8.81kcal/mol; (**b**) **3D** view of interaction between Glucocapparin and the Nucleoprotein of Crimean Congo hemorrhagic fever virus.

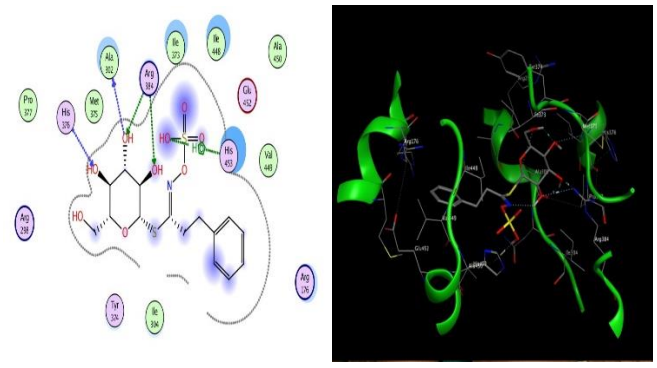
3.2.2. GLUCONASTURTIIN

The phytochemical Gluconasturtiin also show fair interaction with the OTU protease and Nucleoprotein. This phytochemicals interacts with the OTU protease at the amino acid no, 139, 141, 157, 162 and 166 (Figure 3). In the same way, it interacts with the Nucleoprotein at the amino acid no, 302, 376, 384 and 453 (Figure 4). Gluconasturtiin show quite low binding energies with the target proteins that is -12.96 and -7.41 respectively.



(a) (b)

Figure 3. Interaction of Gluconasturtiin from broccoli with OTU protease of Crimean Congo hemorrhagic fever virus. (**a**) **2D** view of Interaction between Gluconasturtiin and the OTU protease of Crimean Congo hemorrhagic fever virus. Interaction has been on the amino acid no, 139, 141, 157 and 166. The binding energy of the ligand during the docking process was -12.96kcal/mol; (**b**) **3D** view of interaction between Gluconasturtiin and the OTU protease of Crimean Congo hemorrhagic fever virus.

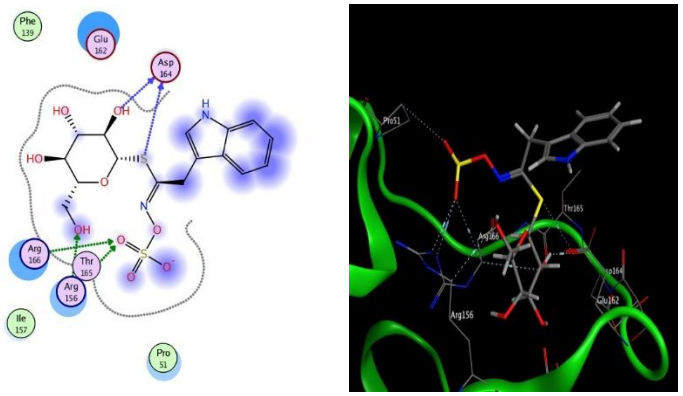


(a) **(b)**

Figure 4. Interaction of Gluconasturtiin from broccoli with the nucleoprotein of Crimean Congo hemorrhagic fever virus. (**a) 2D** view of interaction between Gluconasturtiin and the Nucleoprotein of Crimean Congo hemorrhagic fever virus. Interaction has been on the amino acid no, 302, 376, 384 and 453. The ligand has the weight 423.46 g/mol and the binding energy of the ligand during the docking process was -7.41kcal/mol; (**b**) **3D** view of interaction between the Gluconasturtiin and the Nucleoprotein of Crimean Congo hemorrhagic fever virus.

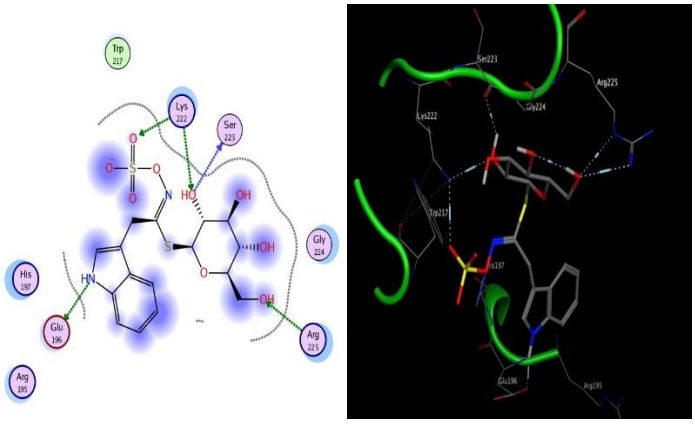
3.2.3. Glucobrassicin

Like Glucocapparin and Gluconasturtiin, Glucobrassicin showed fair interaction with both OTU protease and Nucleoprotein with lowest binding energies. Glucobrassicin interacts with the OTU protease at the amino acids no 156, 164, 165 and 166 respectively (Figure 5). Glucobrassicin also interacts with the active site of Nucleoprotein at the amino acid no, 202 and 237 (Figure 6). This phytochemicals interacts with the target proteins at very low binding energies i-e binding energy of the phytochemical with OTU protease is -9.0kcal/mol. Similarly binding energy of the phytochemical with the Nucleoprotein is -11.74kcal/mol.



(a) (b)

Figure 5. Interaction of Glucobrassicin from broccoli with the OTU protease of Crimean Congo hemorrhagic fever virus. (**a**) **2D** view of interaction between Glucobrassicin and the OTU protease of Crimean Congo hemorrhagic fever virus. Interaction has been on the amino acid no, 156, 164, 165 and 166 respectively. The ligand has the weight 447.46 g/mol and the binding energy of the ligand during the docking process was -9.0kcal/mol; (**b**) **3D** view of interaction between Glucobrassicin and the OTU protease of Crimean Congo hemorrhagic fever virus.



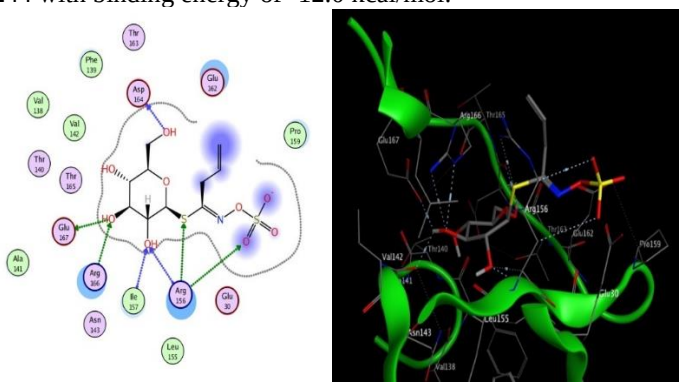
(a) (b)

Figure 6. Interaction of Glucobrassicin from broccoli with the Nucleoprotein of Crimean Congo hemorrhagic fever virus. (**a**) **2D** view of interaction between Glucobrassicin and the Nucleoprotein of Crimean Congo hemorrhagic fever virus. Interaction has been on the amino acid no, 196, 222, 223 and 225 respectively. The ligand has the weight 447.46 g/mol and the binding energy of the ligand during the docking process was -10.11kcal/mol; (**b**) **3D** view of interaction between Glucobrassicin and the Nucleoprotein of Crimean Congo hemorrhagic fever virus.

3.2.4. Sinigrin

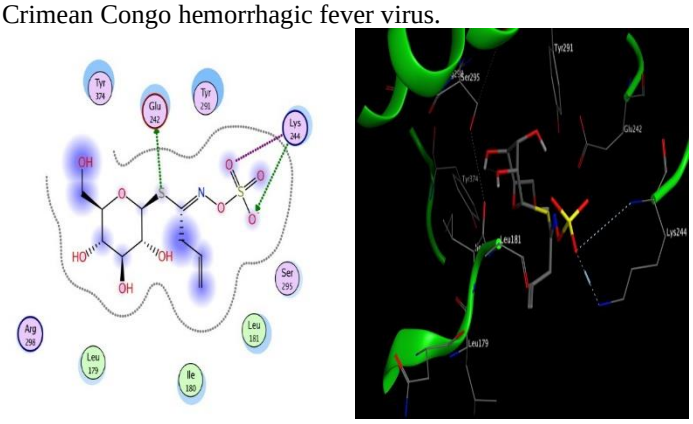
Sinigrin is another member of the class glucosinolate. Sinigrin show fair interaction with both the OTU protease and the Nucleoprotein. Upon docking, Sinigrin shows interaction with the OTU protease at the amino acid no, 156, 157, 164, 166 and 167 (Figure 7). Interestingly the binding energy is very low here. Binding energy of Sinigrin with the OTU protease is -14.18kcal/mol. Sinigrin also shows interaction with the

Nucleoprotein of Crimean Congo hemorrhagic fever virus. It interacts with the Nucleoprotein at the amino acid no, 242 and 244 with binding energy of -12.0 kcal/mol.



(a) (b)

Figure 7. Interaction of Sinigrin from broccoli with the OTU protease of Crimean Congo hemorrhagic fever virus. (**a**) **2D** view of interaction between Sinigrin and the OTU protease of Crimean Congo hemorrhagic fever virus. Interaction has been on the amino acid no, 156, 157, 164, 166 and 167 respectively. The ligand has the weight 358.37 g/mol and the binding energy of the ligand during the docking process was -14.18kcal/mol. (**b**) **3D** view of interaction between Sinigrin and the OTU protease of Crimean Congo hemorrhagic fever virus.



(a) (b)

Figure 8. Interaction of Sinigrin from broccoli with the Nucleoprotein of Crimean Congo hemorrhagic fever virus. (**a**) **2D** view of interaction between Sinigrin and the Nucleoprotein of Crimean Congo hemorrhagic fever virus. Interaction has been on the amino acid no, 222 and 224 respectively. The ligand has the weight 358.37 g/mol and the binding energy of the ligand during the docking process was -12.0kcal/mol; (**b**) **3D** view of interaction between Sinigrin and the Nucleoprotein of Crimean Congo hemorrhagic fever virus.

3.3. Docking of the resultant phytochemicals with similar human protein

The phytochemicals showing fair interaction with the OTU protease and Nucleoprotein when docked with the Human DNA polymerase Lambda Protein. This step was taken in order to know whether these phytochemicals will make interaction with human protein or not. Fortunately none of the phytochemicals made interactions neither docked with the Human DNA polymerase Lambda except the Gluconasturtiin, which is binding to the Human DNA Polymerase Lambda with a binding energy of -7kcal/mol. But this value is quite large as of Gluconasturtiin binds to the OTU protease of Crimean Congo hemorrhagic fever virus at a very low binding energy i-e -12.96 kcal/mol.

3.4. Comparison of the selected phytochemicals as inhibitor with the former drug Ribavirin

Most of the phytochemicals of the broccoli plant showed fair interaction with the OTU protease with lesser binding energies as compared to the former synthetic drug Ribavirin.

The phytochemicals Glucocapparin, Gluconasturtiin, Glucobrassicin and Sinigrin showed better compatibility with the OTU protease with lesser binding energies than its former drug Ribavirin. In Table 1 a brief comparison is made between the former drug Ribavirin and the screened phytochemicals docked with the OTU protease.

Table 1. Comparison between Ribavirin and the compatible screened phytochemicals upon docking with OTU protease of Crimean Congo hemorrhagic fever virus.

	Binding energy kcal/mol	**No, of interaction**	**Log P**	**Lof S**	**Weight gm/mol**
Ribavirin	-10.89	5	-2.92	0.47	244.21
Glucocapparin	-12.69	4	-2.33	-0.7	333.34
Gluconasturtiin	-12.96	4	-0.71	-2.4	423.46
Glucobrassicin	-9.0	5	-0.97	-2.88	447.47
Sinigrin	-14.1	7	-2.11	-1.45	358.37

It is clear from the above comparison that on the basis of lowest binding energies and fair interactions, the phytochemicals (Glucosinolates); Glucocapparin, Gluconasturtiin, Glucobrassicin and Sinigrin can be used as inhibitors of the OTU protease and the Nucleoprotein of Crimean Congo hemorrhagic fever virus instead of the synthetic drug Ribavirin.

DISCUSSION

The basic proteins of a pathogen or the cytotoxic factor which is inducing the disease are of great important in designing new drugs against the specific pathogen [12]. Knowledge of the interactions of these cytotoxic factors with phytochemicals help in identifying potential new drugs for future use in controlling the disease effectively [13, 14].

Sequence analysis of the selected domain and the protein i-e OTU protease and Nucleoprotein of Crimean Congo hemorrhagic fever virus gives us a clear idea about its similarity with the nearest group pathogens. When the sequences of the nearest group pathogens was downloaded from NCBI and was then aligned through the MEGA6 software, it showed us that the OTU protease of Dugbe virus, Hazara virus and Nairobi sheep

disease virus has 18.37% of homology with the OTU protease of Crimean Congo hemorrhagic fever virus. In the same way the nucleoproteins from viruses like Dugbe virus, Hazara virus and Nairobi sheep disease virus showed 41.71% homology with nucleoprotein of Crimean Congo hemorrhagic fever virus.

Plants have been extensively used as a source of new drugs for human diseases and there are several reports on finding drugs from this treasure for previously incurable infections [15, 16]. Among the huge variety of phytochemicals, there exist compounds which may act as potent drugs with least side effects [17]. Synthetic drugs on the other hand being unnatural have a number of side effects making them unsuitable for use in some patients [18]. In order to find out phytochemicals which could inhibit the Congo viral OTU protease and protein (Nucleoprotein), and replace the synthetic inhibitor ribavirin this in-silico study was conducted. From literature we figured out two basic protein of the Crimean Congo hemorrhagic fever virus both of which have the most elementary function in the replication of Crimean Congo hemorrhagic fever virus and degradation of host DNA. RNA Dependent RNA Polymerase has a basic role in synthesizing new strands. In the same way the nucleoprotein of Crimean Congo hemorrhagic fever virus is known for having the DNA specific endonuclease activity [19]. Targeting these two proteins we tried to find out phytochemicals which could serves as inhibitors for these proteins.

Phytochemicals of Broccoli plant (Brassica olearaceae var. italica) and other members of brassicaceae were screened for interaction with the selected proteins of Crimean Congo hemorrhagic fever virus. Broccoli plant has been known for having efficient phytochemicals which could help human body in many drastic conditions [20]. A number of phytochemicals including Glucocapparin, Glucoraphanin, Gluconasturtiin, Glucobrassicin, Sinigrin, Sulforaphane, Amorfrutin, Indol-3-carbinol, Indol-3-ylcarbinol, phenylethyl isothiocynate, Iso-thiocynates and S-Methyl Cysteine Sulfoxide interacted with the active side of the selected proteins. Usually when a ligand binds to a protein the conformation of the protein changes and hence the structure of the protein is altered. The conformation of the protein determines a protein normal functionality so by changing conformation of the protein, a ligand indirectly affect the normal functions of the protein [21-24]. It is also thought that proteins are allosteric in nature. Each protein can adopt two or more conformation when a ligand attaches to it. This phenomenon is not only for the enzymes but all the existing proteins including receptors, structural and motor proteins. When a protein shifts from one conformation to another, its functionality changes [25]. To form stable complex with the target protein the desirable phytochemical is supposed to bind to the active site of the protein with lowest binding energies [26]. It is due to the fact that they do not need energy instead they give energy to the system. Therefore drugs with more negative values of binding energy and greater number of interactions are considered to be more efficient. The above methodology may be suitable as a screen for candidate inhibitors that can then be tested using in vitro assays to see if they inhibit virus replication in cell culture.

CONCLUSION

This whole study was conducted for designing novel drug against CCHF. Due to activeness against many pathogenic diseases, we selected the broccoli plant whose phytochemicals were screened by the docking process. Most of the phytochemicals of the Broccoli plant interacted with the target proteins. Due to their fair interactions with the OTU protease and Nucleoproteins and lowest binding energies, the members of class Glucosinolates i-e Glucocapparin, Gluconasturtiin, Glucobrassicin and Sinigrin may be used as a potential inhbitors against the OTU protease and nucleoprotein of CCHFV. Interactions of these phytochemicals with the targeted domain and protein, obeying Lipinski's rule and their lowest binding energies upon docking are enough for them to be strong inhibitors. Inhibiting the CCHFV OTU protease domain will not directly interfere with the viral replication [27], however it will enable the inate immune system to work efficiently against the pathogen. This whole study would greatly facilitate in future drug designing against CCHFV.

Conflicts of interest

There was no conflict of interest.

Financial statement

No funding was given by any authorities; it was a project thesis of bachelor in science.

Data availability

Data will be provided on demand by corresponding author.

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AUTHORS

First Author – Hamza Bacha, Master's in Botany,
Abdul Wali Khan University Mardan.
Hamza_bacha@awkum.edu.pk

Second Author – Dr. Anwar Hussain, Ph.D. (Botany),
Abdul Wali Khan University Mardan.
drhussain@awkum.edu.pk

Third Author – Sufaid Khan, Master's in Botany,
Abdul Wali Khan University Mardan.
Sufaid@awkum.edu.pk

Fourth Author – Nizar Nawaz, Master's in Botany,
Abdul Wali Khan University Mardan.

Fifth Author – Majid Khan, Master's in Botany,
Abdul Wali Khan University Mardan.
Majidkhan.botany@gmail.com

Corresponding author– Hamza Bacha, Master's in Botany,
Abdul Wali Khan University Mardan.
Hamza_bacha@awkum.edu.pk

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In silico screening of phytochemicals from Brassicaceae family as potential antiviral drugs against Crimean-Congo hemorrhagic fever