RESEARCH PAPER

Genomic and Proteomic Analysis of Sars Cov for Exploring Its Herbal Remedies Through Molecular Docking

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ABSTRACT

The novel coronavirus (2019-nCoV) has been recently identified in patients who are suffering from acute respiratory disease. The novel coronavirus SARS-CoV-2, first identified in Wuhan, China in 2019, is genetically related to SARS-CoV, which caused the 2002-2003 severe acute respiratory syndrome outbreak. The decade-long studies on finding the structural receptors of SARS-CoV have shown key players like - SARS-CoV spike protein (2GHV), host receptor angiotensin-converting enzyme 2 (ACE2) (1R4L), the RNA binding domain of N-protein from SARS (2OG3), and COVID-19 main protease (6LU7) which are responsible for the regulation of the cross-species as well as human-to-human transmissions of SARS-CoV. A large pool of diverse herbal compounds can be found in the traditional medicines of several Asian countries, which are still very much entrusted over the modern allopathic medicines. These first-line treatments show great therapeutic activities including antiviral activities with low cost and negligible side-effects. This study aims to estimate and assess the antiviral potential of these easily available herbal compounds against human coronavirus infections using molecular docking techniques. In the current study, 5 potential antiviral compounds were selected through intense literature studies. The molecular docking of all the 5 selected herbal compounds was done against 4 target proteins (2GHV, 1R4L, 2OG3 & 6LU7) using AutoDock Vina, to study the comparative interaction between the selected ligands and target proteins. Molecular docking using AutoDock Vina revealed that Amentoflavone exhibited the strongest binding affinity with ACE2 (-15.1 kcal/mol), suggesting potential inhibitory activity. Though the results show that compound Amentoflavone proved to be most promising against the human coronavirus, the other compounds were also showing favourable results against the COVID-19. These studies can help in exploring more such herbal compounds against viruses of the corona family, so that further in vitro studies can be carried out in near future.

Keywords: COVID-19, SARS-CoV, spike protein, ACE2, herbal, Amentoflavone.

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INTRODUCTION

The new coronavirus has evolved into a global pandemic, referred to as COVID-19 by the World Health Organisation (WHO). The current outbreak of the coronavirus is attributed to a newly identified strain of the severe acute respiratory syndrome coronavirus, known as SARS-CoV-2. Coronaviruses (CoVs) have the capacity to infect both animals and humans. The virus in question is classified under the family Coronaviridae,

specifically the subfamily Coronavirinae. It has a positive-sense single-stranded ribonucleic acid (RNA) genome. Coronaviruses (CoVs) possess a genome consisting of single-stranded, positive-sense RNA and are classified into four genera, namely α-, β-, γ-, and δ-coronaviruses[1]. The nomenclature of this virus is derived from its genetic relationship to the virus responsible for the 2003 SARS epidemic, although they exhibit distinct characteristics. Following this, the World Health Organisation (WHO) officially designated the term "COVID-19" for the novel illness[2]. However, the emergence of severe acute respiratory syndrome (SARS) in 2003, caused by the SARS-Cov coronavirus agent belonging to the betacoronavirus subfamily, prompted an immediate need for study on coronaviruses associated with SARS. SARS-CoV-2 is classified as an enveloped RNA virus belonging to the betacoronavirus genus[3]. The current pandemic of COVID-19, caused by the SARSCoV-2 virus, was first detected in Wuhan City, located in the Hubei province of southern mainland China, on December 31, 2019, the genetic makeup of SARS-CoV-2 has an estimated 70% similarity with that of SARS-CoV[4].

The SARS-CoV virus possesses specific structural receptors, such as the SARS-CoV spike protein (2GHV), the host receptor angiotensin-converting enzyme 2 (ACE2) (1R4L), the RNA binding domain of the N-protein from SARS (2OG3), and the COVID-19 main protease (6LU7). These receptors play a crucial role in governing the transmission of SARS-CoV across different species and facilitating human-to-human transmission. These receptors play a significant role in the global spread of the epidemic. As time progresses, while a vaccine has been developed, concerns over the persistence of the pandemic remain. The spike protein (2GHV) is responsible for the reproduction of the virus inside host cells. The interaction between the spike protein and the receptor protein on the host cell, known as angiotensin-converting enzyme 2 (ACE2) (1R4L), facilitates viral infection[5]. The RNA-binding N protein is an essential component for the processes of viral RNA transcription and replication. The packaging of the viral RNA genome, RNA synthesis in replication or transcription, and the regulation of infected cell metabolism are all essential functions performed by this entity. The global community is now grappling with a significant challenge pertaining to a substantial increase in mortality rates. The efficacy of immunisations does not reach 100%. Furthermore, in light of the advent of novel viral strains, including more mutated variants, researchers continue to grapple with determining the efficacy and potential negative effects associated with the administration of vaccinations.

Following the first occurrence of COVID-19 in India, which was officially reported on January 30th, 2020. Over the course of a two-year period, the coronavirus strains have shown an increasing level of potency and resistance, mostly owing to the emergence of novel variations such as the Delta variant and the Omicron variant. It is worth noting that the current vaccinations may not possess complete efficacy against these aforementioned variants. The typical respiratory symptoms seen in those who are sick include elevated body temperature, persistent coughing, difficulty breathing, and experiencing a sensation of breathlessness. In instances of heightened severity, infection has the potential to induce pneumonia, severe acute respiratory syndrome, renal failure, and fatality[6]. In recent instances of the coronavirus illness, it has been shown that discernible symptoms are often absent until a critical stage has been reached, rendering medical intervention ineffective. Therefore, the combination of a compromised immune system and the limited availability of antiviral medications present a formidable obstacle to ongoing worldwide endeavours aimed at mitigating the spread of the COVID-19 pandemic[7].

Traditional medicines in several Asian nations include a wide range of herbal ingredients, which continue to be highly valued in comparison to contemporary allopathic medications. Several studies have demonstrated the antiviral properties of certain herbal medicines against a range of virus strains, including coronavirus, herpes simplex virus, influenza virus, human immunodeficiency virus, and hepatitis B and C viruses[8-10]. The five herbal chemicals that were discovered following an extensive literature search are Amentoflavone, Resveratrol, Catechin gallate, Artemisinin, and Aloe emodin. The use of herbal components enables the administration of initial therapy options that exhibit significant therapeutic efficacy, particularly in terms of antiviral properties. Moreover, these therapies are characterised by their cost-effectiveness and the low occurrence of adverse effects[11-15].

Amentoflavone exhibits properties that contribute to its efficacy as an antioxidant[16], anti-inflammatory agent[17], and anti-tumorigenic compound, as shown by its reported effectiveness against cancer[18]. The anti-virus has shown inhibitory effects on several viruses, including the dengue virus, HIV, and SARS-CoA[19]. Additionally, it has been have reported its antifungal properties as well as its potential applications in the central nervous system and cardiovascular system[19]. Resveratrol has been shown to have potential therapeutic effects against Alzheimer's disease, cancer, diabetes, cardiovascular disorders, and viral infections. Catechin gallate has been shown to have potential therapeutic effects against several conditions, including cancer, Alzheimer's disease, viral infections, and other ailments[20]. Artemisinin has notable anti-inflammatory, antioxidant, and antibacterial characteristics, making it very efficacious in combating malaria[21]. Aloe emodin has potent anti-inflammatory and antioxidant properties, which have shown promise in the potential treatment of several ailments such as cancer, osteoporosis, cardiovascular diseases, central nervous system disorders, liver issues, metabolic disorders, and respiratory illnesses. The substance has antibacterial, antiviral, and antifungal characteristics[22-25].

The objective of this research is to assess the antiviral efficacy of readily accessible herbal substances against human coronavirus infections via in silico methodologies. The objective of this study is to use molecular docking methods in order to quantify and evaluate the antiviral efficacy of certain herbal components against human coronavirus infections. The objective is to evaluate the interaction and compare the binding affinities of these herbal medicines with several crucial proteins associated with COVID-19. The interaction between the target proteins and the discovered herbal components was assessed by the use of AutoDock Vina for molecular docking analysis. The comparative interaction between the selected ligands and target proteins was studied by performing molecular docking of the five chosen herbal compounds against four target proteins (2GHV, 1R4L, 2OG3, and 6LU7) using AutoDock Vina. In order to enhance our comprehension of the molecular docking interaction between herbal compounds and proteins, it is important to identify the active binding site of the protein. Hence, via more research and validation, it is plausible that these herbal compounds might be used as efficacious agents against COVID-19, thereby benefiting a substantial populace due to their affordability, accessibility, and absence of adverse reactions.

MATERIALS AND METHODS

The literature survey was done for identification of the key player proteins for the structural receptors of COVID-19, further the responsible protein was studied through UNIPROT database. The structure and PDB file of protein was done using Protein Data Bank. The Blastp was done to identify the conserved region and the superfamily of protein for further its functional analysis.

The novel compounds for the effective treatment of SARS-CoV were identified through literature survey. The interactions of these compounds against the protein molecules of SARS-CoV were studied using molecular docking. The novel compounds were saved in SDF file downloaded from PUBCHEM database for molecular docking study.

The AutoDock Vina Software was used for studying the molecular docking interaction between ligand and protein. The methodology used for the current study is shown in figure 1.

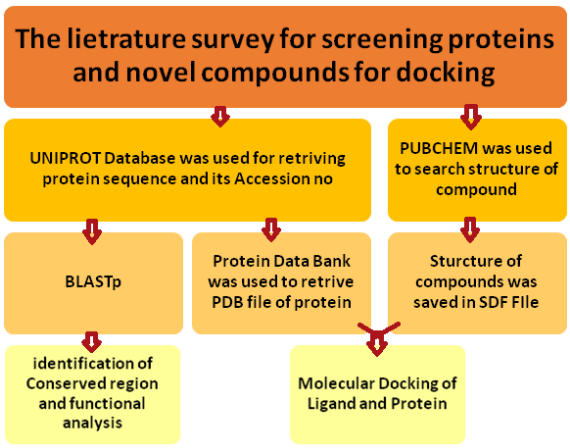


Figure 1: Steps showing methodology followed for the current study

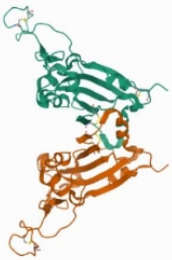
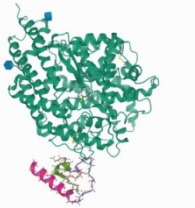
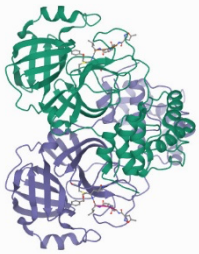
RESULTS

Literature survey for identification of the key structural receptors' proteins of COVID-19

The structural receptors of COVID-19 have shown that the key players proteins are SARS-CoV spike protein (2GHV), host receptor angiotensin-converting enzyme 2 (ACE2) (1R4L), the RNA binding domain of N-protein from SARS (2OG3), and COVID-19main protease (6LU7), which are responsible for the regulation of the cross-species

as well as human-to-human transmissions of COVID-19 as shown in Table 1.

Table 1: Key player proteins chosen as structural receptors of COVID-19 for this study and their structures

S. No.	Receptor proteins	PDB ID	Structure
1.	Spike protein	2GHV	
2.	Host receptor angiotensin-converting enzyme 2 (ACE2)	1R4L	
3.	RNA binding domain of N-protein from SARS	2OG3	
4.	COVID-19 main protease	6LU7	

Genomic and functional analysis of selected receptor proteins

Spike Glycoprotein: The Spike glycoprotein is a crucial component of the SARS-CoV-2 virus responsible for COVID-19. It plays a central role in the infection process by binding to the ACE2 receptor on human cells, facilitating viral entry. The conserved regions of the spike gene are typically found in regions involved in receptor binding and membrane fusion, as these functions are critical for viral entry and are therefore less prone to mutation.

Leukotriene B4 receptor 1: This receptor, also known as BLT1, is primarily associated with the host immune response. It has been suggested that it may play a role in the inflammatory response seen in COVID-19 patients. While the receptor itself may not be directly targeted by the virus, the downstream signalling pathways it influences could impact the immune response. Conserved regions in its gene may relate to its role in normal immune function.

Nucleoprotein: The nucleoprotein of SARS-CoV-2 is responsible for binding to the viral RNA genome, forming the ribonucleoprotein complex essential for viral replication and transcription. Conserved regions in the nucleoprotein gene are often found in RNA-binding domains, ensuring the virus maintains its ability to replicate and transcribe its RNA genome accurately.

Replicase polyprotein 1ab: This polyprotein contains several non-structural proteins, including RNA-dependent RNA polymerases and proteinases responsible for processing the viral polyprotein into functional components. The conserved regions in the replicase polyprotein gene are critical for maintaining the virus's ability to replicate its RNA genome and produce functional proteins necessary for viral assembly and infection.

Genomic analysis of the Spike Glycoprotein can reveal mutations affecting ACE2 receptor binding and conformational changes, crucial for vaccine development and understanding viral adaptability. Investigating Leukotriene B4 Receptor 1 variations helps grasp its role in COVID-19 inflammation and guides potential therapies to modulate the immune response. Nucleoprotein analysis uncovers RNA-binding mutations and viral interactions, aiding in drug target discovery. Examining Replicase Polyprotein 1ab mutations sheds light on their impact on viral replication and processing, offering potential antiviral drug targets as shown in Table 2.

Table 2: Genomic and Functional Analysis of Selected Receptor Proteins

S. No.	Gene	Protein	Organism	Protein function	Conserved region (Superfamily)	Accession no.
1.	S	Spike glyco	Severe acut	Spike protein S1	CoV_Spike_S1_RBO	P59594

		protein	e respiratory syndrome coronavirus (SARS-CoV)	initiates infection and induces S glycoprotein conformational changes, while Spike protein S2 mediates viral membrane fusion, host tethering down-regulation, ACE2/CLEC4M/DC-SIGNR binding for internalization, and cathepsin CTSL-driven membrane fusion within endosomes.		
2.	LTB4R	Leukotriene B4 receptor 1	Homo sapiens (Human)	This receptor is involved in extracellular ATP, UTP, and ADP signalling, mediating its activity through G proteins and a phosphatidylinositol-calcium second messenger system, potentially influencing cardiac muscle contraction and serving as a receptor for leukotriene B4 in inflammation and immune responses.	7tm_GPCRs	Q15722
3.	N	Nucleoprotein	Severe acute respiratory syndrome coronavi	It packages viral RNA, aids in virion assembly, enhances RNA transcription	CoV_N-NTD	P59595

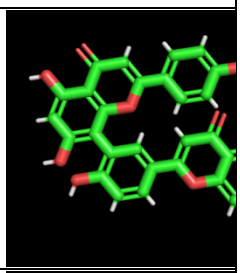
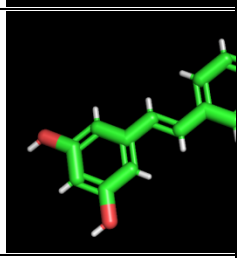
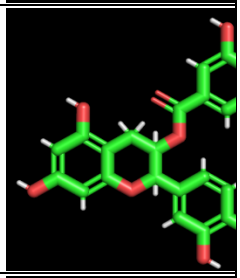
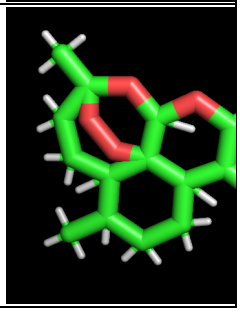
			rus (SARS-CoV)	and replication, and potentially influences transforming growth factor-beta signalling by binding to host factors.		
4.	rep	Replicase polyprotein 1ab	Severe acute respiratory syndrome coronavirus 2 (2019-nCoV) (SARS-CoV-2)	This multifunctional protein is essential for viral RNA transcription and replication and contains proteinases responsible for polyprotein cleavage.		P0DTD1

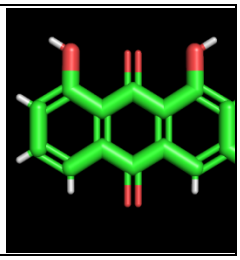
Screening and identification of anti-viral herbal compounds

The 5 herbal compounds identified through intensive literature search were Amentoflavone, Resveratrol, Catechin gallate, Artemisinin and Aloe emodin. The basis for screening antiviral these herbal compounds for docking against COVID-19 proteins lies in their potential to contain bioactive molecules with known antiviral properties. These compounds were selected based on their historical use in traditional medicine, prior studies suggesting antiviral effects, or their ability to target specific viral proteins involved in the infection and replication cycle of the SARS-CoV-2 virus. Docking studies can predict how these compounds interact with viral proteins, providing valuable insights into their potential as therapeutic agents against COVID-19.

The structure of all the screened compounds was searched from PubChem and was saved in SDF file format for further molecular docking analysis. The details of the compounds are mentioned in Table 3.

Table 3: Identified anti-viral herbal compounds

S. No.	Herbal compound	PubChem ID	Structure
1.	Amentoflavone	CID_5281600	
2.	Resveratrol	CID_445154	
3.	Catechin gallate	CID_6419835	
4.	Artemisinin	CID_68827	

5.	Aloe emodin	CID_10207	

Molecular docking interaction studies

The highest binding energy ΔG was observed for Amentoflavone with -15.1 kcal/mol against host receptor angiotensin-converting enzyme 2 (ACE2) protein (1R4L) as shown in Table 4. Amentoflavone has shown highest binding energy with all the selected protein of SARS CoV, among other herbal compounds. Though all 5 herbal compounds were showing effective docking energy score with all the selected proteins, the receptors of SARS-CoV. The binding sites and amino acid residues involved in the interaction of the protein with the ligands is shown in Table 5. The Gly267, Arg517 are the amino acid residue sites at which the docking interaction was observed with Amentoflavone. Tryptophan, Threonine, Alanine, Glycine, Arginine, Aspartic acid, Lysine, Serine, Histidine, Asparagine, Tyrosine, Valine, Isoleucine and Glutamine are amino acid residues of selected proteins receptors, which are the active binding sites for all the selected 5 herbal compounds. Arginine and Aspartic acid are the major identified amino acids, which were highly involved in protein-ligand interaction.

Table 4: Comparative docking energies of selected proteins with identified herbal compounds

S. No.	**Ligand for molecular docking against 2019-nCoV protein**	**Binding energy ΔG (kcal/mol)**			
		Spike protein (2GHV)	**ACE 2 (1R4L)**	**RNA binding domain of N-protein from SARS (2OG3)**	**COVID-19 main protease (6LU7)**
1.	Amentoflavone	-12.3	**-15.1**	-12.7	-11.4
2.	Resveratrol	**-8.0**	-7.7	-7.2	-6.6
3.	Catechin gallate	-10.3	**-10.5**	-8.8	-8.6
4.	Artemisinin	-9.1	**-9.9**	-8.9	-9.2
5.	Aloe emodin	**-8.5**	-8.3	-7.1	-7.7

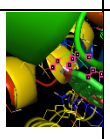
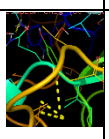
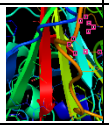
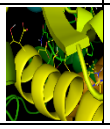
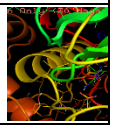
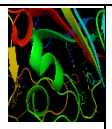
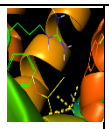
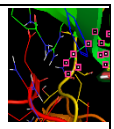
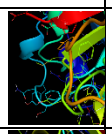
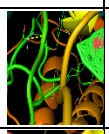
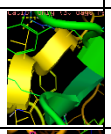
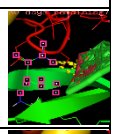
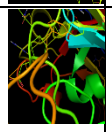
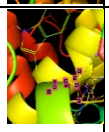
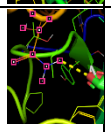
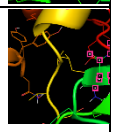
Table 5: Amino acid residues showing interaction with selected herbal compounds

S. No.	**Ligand for molecular docking against 2019-nCoV protein**	**Amino acid residue positions**			
		Spike protein (2GHV)	**ACE 2 (1R4L)**	**RNA binding domain of N-protein from SARS (2OG3)**	**COVID-19 main protease (6LU7)**
1.	Amentoflavone	Thr358, Try422	Gly267, Arg517	Arg66, Arg69, Asp126	Glu109, Asp152, Ser153
2.	Resveratrol	Arg440, His444, Ser455	Lys352	Ser78, Tyr111, Tyr172	His163, Thr189, Glu191
3.	Catechin gallate	Arg440, Arg442, Asp456	Asp381, Arg513	Isoleu85, Asp126, Val131	Glu109, Glu110, Asp152, Ser153
4.	Artemisinin	Arg440, Ser455, Gly402	Arg517	Asp76, Thr157	Glu109, Asp152
5.	Aloe emodin	Thr358,	Try326,	Arg69,	Glu109,

		Try422	Thr333, Ala347	Asp140	Asp152, Ser153

Amino acid residues within COVID-19-causing selected proteins are critical in elucidating the interaction dynamics with selected herbal compounds via docking studies. By identifying these key residues, researchers gain insights into the precise binding sites and affinity of herbal compounds for viral proteins. The identified amino acid residues and the binding interaction sites of herbal compounds with target proteins is documented in Table 5 and Table 6. This information is invaluable for rational drug design and development, as it aids in predicting the effectiveness of herbal compounds as potential antiviral agents. Understanding the molecular interactions at the amino acid level enables the fine-tuning of compounds to optimize their binding affinity and specificity, ultimately leading to the design of more potent and targeted therapies to disrupt viral protein function. This approach holds great promise in the search for effective treatments against COVID-19.

Table 6: Binding interaction sites of herbal compounds with target proteins

S. No.	**Ligand for molecular docking against 2019-nCoV protein**	**Binding interaction sites**			
		Spike protein (2GHV)	**ACE2 (1R4L)**	**RNA binding domain of N-protein from SARS (2OG3)**	**COVID-19 main protease (6LU7)**
1.	Amentoflavone				
2.	Resveratrol				
3.	Catechin gallate				
4.	Artemisinin				
5.	Aloe emodin				

The current global COVID-19 epidemic has brought attention to the pressing need for the development of efficacious medicines targeting the virus. The potential antiviral effects of herbal substances have garnered significant research. This work used molecular docking techniques to examine the binding relationships of five herbal medicines (Amentoflavone, Resveratrol, Catechin gallate, Artemisinin, and Aloe emodin) and four key protein targets linked to the SARS-CoV-2 virus. The findings of our study demonstrate encouraging binding affinities and provide insights into possible methods by which these chemicals may be effective in treating the COVID-19 virus.

The worldwide health catastrophe induced by the SARS-CoV-2 virus, often known as the COVID-19 pandemic, has compelled the expeditious development of antiviral therapies. The study of traditional medicine, including herbal medicines, has been undertaken to examine its potential as a source of innovative therapeutic alternatives. The computer approach known as molecular docking has emerged as a crucial tool in the field of drug development, allowing for the prediction of interactions between ligands and proteins.

Molecular docking simulations were conducted utilising advanced docking software (please specify the software) to evaluate the binding affinities between herbal compounds and four protein targets, namely the spike protein (2GHV), ACE2 (1R4L), the RNA binding domain of the N-protein from SARS (2OG3), and COVID-19 main protease (6LU7). The calculation of the binding energies (ΔG) between the ligands and protein targets was performed.

The docking results have provided fascinating observations on the prospective antiviral characteristics of the herbal medicines. The binding affinities of all five herbal compounds

were shown to be beneficial when interacting with the protein targets. Amentoflavone consistently exhibited the highest affinity for binding, indicating its potential as a wide-ranging antiviral therapeutic drug. The compounds Amentoflavone and Artemisinin exhibited significant interactions with the major protease (6LU7) of the COVID-19 virus, suggesting their potential as inhibitors of viral replication. Amentoflavone, Artemisinin, and Catechin gallate shows significant interactions with the RNA binding domain of the N-protein from SARS (2OG3), indicating a potential involvement in disrupting viral RNA mechanisms. The interference of the interaction between the spike protein and ACE2 is of utmost importance in the prevention of viral entry. Amentoflavone, Catechin gallate, and Artemisinin exhibited notable binding affinities towards ACE2 (1R4L), suggesting their potential as inhibitors of viral entry. The binding interactions found between the herbal components and the target proteins provide valuable insights into the underlying mechanisms. One example of a compound that has the potential to interfere with the viral replication process is resveratrol. This compound is believed to disrupt the replication cycle by interacting with key components such as the major protease and the spike protein.

This research is of utmost significance and represents a critical milestone in the pursuit of an improved treatment for COVID-19, owing to numerous compelling factors. The use of *in silico* investigations, such as the one described, offers an expeditious and economically efficient approach to finding prospective drug candidates. The results have the potential to accelerate the development of efficacious therapies for COVID-19. The herbal substances demonstrated a range of binding affinities towards various protein targets, indicating the presence of multifarious mechanisms that might potentially be used in a combination treatment strategy. Certain herbal components have been identified to possess antiviral activity against certain illnesses. The current work offers a potential avenue for the repurposing of drugs, thereby expediting the progression towards clinical trials. The computational insights have the potential to lead to specific experimental studies, thereby decreasing the burden of conducting extensive experiments. However, it is important to note that further experimental validation is still necessary.

This work demonstrates the potential of five herbal components as antiviral medicines against COVID-19 via the use of molecular docking simulations. The binding affinities and interactions between the discovered compounds and crucial protein targets serve as a fundamental basis for further investigations, which may ultimately result in the formulation of efficacious therapeutic approaches for the current global pandemic. This study highlights the significance of multidisciplinary collaboration in the field of drug development and emphasises the use of computational methodologies to efficiently discover prospective therapeutic candidates. This study provides a comparative molecular docking analysis of five bioactive phytochemicals against four key SARS-CoV-2 protein targets, highlighting Amentoflavone as a potential multi-target antiviral candidate.

CONCLUSION

The molecular docking results between the 5 herbal compounds and the selected protein receptors of 2019-nCoV shows great interaction and proves to be highly promising against human corona virus. The active binding site of protein can be identified to better study the interaction of herbal compound with protein during the molecular docking interaction. Therefore, with further studies and verifications, these herbal compounds can be used effectively against COVID-19, helping a large population as they are less costly and easily available with no side-effects. Further comparative *in silico* studies and wet lab verification is required to study and verify the actual effects of these herbal compounds against COVID-19. Novel modification and moderation is required on the basis of wet lab results to make these herbal compounds more effective and efficient.

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Nil.

Conflict of interest

There are no conflicts of interest.

DECLARATIONS

Ethical Approval: This study did not involve human participants or animals. Ethical approval was not required

Data Availability: All data generated or analysed during this study are included in this published article

Confirm Informed Consent: Not applicable

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