International Journal of Life Sciences, Biotechnology and Pharma Research Vol. 14, No. 5, May 2025 Online ISSN: 2250-3137
Print ISSN: 2977-0122

DOI: 10.69605/ijlbpr_14.5.2025.8

ORIGINAL RESEARCH

Profiling of antifungal activity of phytochemicals against the fungal agents effecting okra crops through molecular docking

[1]Anshika Dubey, [2]Mala Trivedi, [3]Prachi Srivastava, [4]Shalini Upadhyay

[1]Postgraduate student, [2]Professor, [3]Assistant Professor, Department of Biotechnology, Amity Institute of Biotechnology, Amity University, Lucknow, Uttar Pradesh, India
[4]Assistant Professor, Department of Microbiology, A.S.J.S.A.T.D.S. Medical College, Fatehpur, Uttar Pradesh, India

Corresponding author
Dr. Shalini Upadhyay
Assistant Professor, Department of Microbiology, A.S.J.S.A.T.D.S. Medical College, Fatehpur, Uttar Pradesh, India
Email: shalini.upd@gmail.com

Received: 29 March, 2025 Accepted: 25 April, 2025 Published: 01 May, 2025

ABSTRACT

Background: Okra a valued vegetable for its economic and nutritional value is often affected by a number of fungal infections having detrimental effect on its production. Powdery mildew, Fusarium wilt, Cercospora leaf spot and Anthracnose are the most common fungal diseases which not only hinder a plant's capacity to grow and produce, but they also make the produce less marketable. This study is an attempt towards procuring a potent phytochemical agent against the common fungal agents affecting okra. **Methods:** In the present study, gene list was gathered from MBGD (Microbial Genome Database for Comparative Analysis) and imported into Cytoscape to create gene network analysis. The "dnaK" gene was identified as the priority gene for phytochemical design construction by Swiss Model. Furthermore, AdMETLab 3.0 was used to screen antifungal phytochemicals based on Lipinski's rule of five. **Results:** Molecular docking done between the phytochemicals and the selected priority gene, revealed the phytochemicals which showed various degree of antifungal activity. Consequently, the results suggest which phytochemicals have antifungal properties that work best and which ones should be combined to create organic fungicides. Among these, the most potent molecule was found to be berberine. **Conclusion:** This is the first study to the best of our knowledge which attempts to decode the antifungal action of berberine on fungal infections of okra. It seeks to promote the sustainable production of ladyfinger and lower the demand for artificial pesticides.

Keywords: Berberine, antifungal agents, fungal infections, non-synthetic chemicals, Powdery mildew, Fusarium wilt, ladyfinger, genomic study, in silico designing.

INTRODUCTION

The cultivation of ladyfinger (*Abelmoschus esculentus*), also known as okra, is widespread in tropical and subtropical regions due to its nutritional and economic value. This crop is rich in vitamins, minerals, and dietary fibre. It is an essential component of diets worldwide and serves as a vital income source for quite a few small-scale farmers.[1] However, the productivity and quality of ladyfinger are often compromised by various biotic stressors, particularly fungal diseases, which pose a significant threat to sustainable agriculture. The vulnerability of ladyfinger to fungal pathogens has prompted extensive research to identify effective management strategies, including the exploration of antifungal phytochemicals derived from plants. These natural compounds are increasingly recognized for their potential to offer environmentally friendly and sustainable alternatives to synthetic fungicides.[2] Among the most common fungal diseases of okra are powdery mildew, fusarium wilt and *Cercospora* leaf spot. These manifests as a white, powdery growth on the surfaces of leaves, stems, and pods, impeding photosynthesis and ultimately leading to defoliation and reduced fruit quality. Such infections not only diminish the aesthetic and market value of the

DOI: 10.69605/ijlbpr_14.5.2025.8

produce but also reduce the overall plant vigour and productivity. Common fungal pathogens affecting ladyfinger have been compiled in the table 1.[2,3,4] The management of fungal diseases in ladyfinger traditionally relies on the use of synthetic fungicides, which, although effective, pose several drawbacks, including the development of resistant strains, environmental pollution, and health hazards to humans and non-target organisms. The growing concerns over these issues have spurred interest in alternative disease control methods that are sustainable and eco-friendly. One promising avenue is the use of antifungal phytochemicals, which are naturally occurring compounds produced by plants as part of their defence mechanisms against pathogens.[2]

Phytochemicals, including phenolics, terpenoids, alkaloids, and saponins, exhibit diverse biological activities, including antifungal properties. These compounds can inhibit fungal growth and development through various mechanisms, such as disrupting cell wall synthesis, interfering with membrane integrity, and inhibiting enzyme activity. Their integration into IPM (Integrated Pest Management) programs can enhance disease control efficacy while reducing reliance on synthetic fungicides. Furthermore, the use of phytochemicals aligns with organic farming principles and contributes to the sustainability of agricultural systems.[5] Despite the promising potential of antifungal phytochemicals, several challenges need to be addressed to ensure their practical application. These include the standardization of extraction methods, the determination of effective concentrations, and the evaluation of their long-term effects on plant health and soil microbiota. Additionally, understanding the molecular mechanisms underlying the antifungal activity of these compounds can facilitate the development of more targeted and effective formulations. In conclusion, the exploration of antifungal phytochemicals represents a significant step towards sustainable disease management in ladyfinger cultivation. The identification of potent compounds from plant sources and their integration into IPM strategies can mitigate the impact of fungal diseases, enhance crop productivity, and promote environmental sustainability. Future research should focus on optimizing extraction techniques, elucidating the modes of action, and evaluating the field efficacy of these natural antifungals to fully harness their potential in agricultural practices.

MATERIALS AND METHODS

Materials

The software used in this study for designing the required phytochemical against fungal infections affecting okra were as follows:

1. Cytoscape

It is a software project branch called open-source is meant to unify expressed high-throughput data and several molecular sequences with biomolecular interaction networks possible. The core program of Cytoscape provided us the necessary tools for organizing and querying network, graphical amalgamation of these networks with expression profiles, phenotypes and various molecular states. Further connecting all information to functional annotation databases. Cytoscape was employed for a comprehensive integration of molecular interaction network data. The usage of annotations supports static hierarchical data like protein-functional ontologies.

2. PubChem

PubChem is the largest free chemical information database on the planet. This software finds compounds, look for identifiers like structure, name, molecular formula, biological activity, toxicity & safety information, physical and chemical properties, and much more. A variety of chemical information may be found in PubChem, such as 2-dimensional and 3D (three dimensional) structures, physical and chemical characteristics, pharmacology, toxicity, bioactivity information, drug target, metabolism, safety and handling, pertinent patents and scientific articles etc. PubChem provides data on a broad range of chemical entities, however most of its material is on small molecules such as miRNAs, siRNAs, carbohydrates, peptides, lipids, chemically modified macromolecules etc. Majority of the chemical databases included in this work were extracted through PubChem.

3. MBGD (Microbial Genome Database for Comparative Analysis)

MBGD helps in comparative genomics by different types of steps such as paralog clustering, motif analysis, ortholog identification, and gene order comparison. It is a workspace system for analysing sequenced microbial genomes. The primary action of MBGD is to generate a table of orthologous gene classifications from precomputed permutations and combinations of all possible relationships among genes using multiple genomes. This software uses automated classification algorithm to provide assistance in establishing unique classification table according to the organisms of interest and other parameters chosen by the user. This tailor-made data can be utilized to carry out various types of comparative analyses such as phylogenetic pattern analysis, gene order comparison and detailed gene structure comparison as used in this study.

4. Seam Dock

The Seam Dock web-service integrates various docking tools within a common framework that enables ligand global/local docking and hierarchical approach blending both for accelerated identification

DOI: 10.69605/ijlbpr_14.5.2025.8

of interaction site. To create 3D visualization of receptor, ligand and docking poses as well as their interactions with the receptor has taken huge efforts. In general, advanced visualization features in conjunction with coherent library allows users to share data with unlimited number of collaborators all over the world during molecular modelling session.

5. NCBI (National Centre for Biotechnology Information)

The National Institute of Biotechnology Access to genetic and biological data is facilitated by information, which advances both research and health. More specifically, NCBI is in charge of creating automated methods for the analysis and storage of data pertaining to genetics, biochemistry, and molecular biology; it also helps the scientific and healthcare communities make use of these databases and software; organizing national and international efforts to collect biotechnology-related data; and conducting research into cutting-edge computer-based data processing tools for the analysis of the structure and function of biologically relevant molecules. Data retrieval systems and computational resources are provided by NCBI for the analysis of GenBank data as well as many other types of biological data.

6. ADMETLab 3.0

It offers a thorough and effective platform for assessing ADMET-related parameters in addition to physicochemical qualities and medicinal chemistry traits needed for drug discovery. Due to its higher performance and greater coverage of ADMET predictions, this platform is among the most widely used ADMET prediction systems, has not only received a great deal of positive feedback from regular users but has also gained respect in the field of AI-driven drug development.

7. SWISS MODEL

This server enables automated comparative modelling of 3D protein structures. It is the one of the most user-friendly web-based automated modelling tools. The template selection, alignment and model construction are done automatically by the server. The understanding of protein function based on the molecular level provided by 3D structures allows designing effective experiments such as infection-related mutation studies, site-directed mutagenesis, structure-based design of targeted inhibitors etc.

Methodology

The flow of activities performed in in silico designing of the antifungal phytochemical has been depicted in figure 1.

Gene identification: The database MBGD was used to identify the genes of fungi causing infection in okra.

Protein– protein network: The gene interactions within biological system and construction of protein – protein interaction network was performed on Cytoscape (Figure 2). The phytochemical screening was based on Lipinski's rule of 5 using ADMETlab 3.0.

Protein modelling: Swiss-Model was used to generate the 3D structure model of "dnaK" and identification of the key hub gene our protein – protein interaction network analysis. This modelling provided insight into the structural details of dnaK.

Library preparation: After generation of a 3D structure from Swiss Model, the library was to obtain the Canonical SMILES and their sources from PubChem.

Molecular modelling: By using the 3D Structure as a Ligand, we used Seamdock for molecular docking to estimate the binding energy of each phytochemical. The purpose of using Seamdock is to find the most suitable phytochemical.

RESULT

The Gene network Analysis identified the "dnak" gene as priority gene from MBGD and constructed a model for "dnak" as ligand using Swiss Model. The findings showed that "dnaK" gene has a significant role to play in okra infections. After retrieving the "dnaK" gene's protein sequence using Cytoscape, the Swiss Model program was utilized to create 3-D protein structures for further docking research. A library including twenty antifungal phytochemicals was created by a review of the literature and data extraction in PubChem. Twenty compounds were obtained from the phytochemical screening using ADMETLab 3.0 and Lipinski's rule of five. The protein modelling and molecular docking studies conducted in between phytochemicals and the "dnaK" gene are as shown in Table 2.

The chemical "Berberine" had the highest negative binding energy (-8.4) and the strongest binding affinity with the protein "dnaK" in Seam Dock molecular docking investigations. It should thus have potent antifungal action. The results of correlation between the designed phytochemicals with their binding energy and amino acid residues have been depicted in Table 3. The results of docking study have been compiled in the table 4 with the 3D structural details of the designed molecules which can be developed into potent antifungals.

Table 1: Common Fungal Diseases in Okra and effective phytochemicals[2,3]

S. no.	Disease	Pathogen	Effective Phytochemicals
1.	Fusarium Wilt	*Fusarium oxysporum*	Quercetin, Kaempferol
2.	Powdery Mildew	Erysiphe cichoracearum, Oidium asteris	Thymol, Carvacrol

DOI: 10.69605/ijlbpr_14.5.2025.8

3.	Cercospora Leaf Spot	*Cercospora abelmoschi*	Berberine, Sanguinarine
4.	Anthracnose	Colletotrichum spp.	Neem oil, Fenugreek saponins
5.	Charcoal Rot	*Macrophomina phaseolina*	Thymol, Clove oil

Table 2. Analysis of protein modelling and molecular docking studies

Phytochemicals	Plant sources	Lipinski Rule	Canonical SMILES
Allicin	*Allium sativum*	Accepted	C=CCSS(=O)CC=C
Curcumin	*Curcuma longa*	Accepted	COC1=C(C=CC(=C1)C=CC(=O) CC(=O)C=CC2=CC(=C(C=C2)O)OC)O
Eugenol	*Syzygium aromaticum*	Accepted	COC1=C(C=CC(=C1)CC=C)O
Thymol	*Thymus vulgaris*	Accepted	CC1=CC(=C(C=C1)C(C)C)O
Cinnamaldehyde	*Cinnamomum verum*	Accepted	C1=CC=C(C=C1)C=CC=O
Carvacrol	*Origanum vulgare*	Accepted	CC1=C(C=C(C=C1)C(C)C)O
Menthol	*Mentha piperita*	Accepted	CC1CCC(C(C1)O)C(C)C
Capsaicin	*Capsicum species*	Accepted	CC(C)C=CCCCCC(=O)NCC1=CC (=C(C=C1)O)OC
Berberine	*Hydrastic canadensis*	Accepted	COC1=C(C2=C[N+]3=C (C=C2C=C1)C4=CC5=C(C=C4CC3)OCO5)OC
Linalool	*Lavandula angustifolia*	Accepted	CC(=CCCC(C)(C=C)O)C
Resveratrol	*Vitis vinifera*	Accepted	C1=CC(=CC=C1C=CC2=CC (=CC(=C2)O)O)O
Gingerol	*Zingiber officinale*	Accepted	CCCCCC(CC(=O)CCC1=CC (=C(C=C1)O)OC)O
Terpinen-4-ol	*Melaleuca alternifolia*	Accepted	CC1=CCC(CC1)(C(C)C)O
Safrole	*Sassafras albidum*	Accepted	C=CCC1=CC2=C(C=C1)OCO2
Alpha-pinene	*Pinus species*	Accepted	CC1=CCC2CC1C2(C)C
Genistein	*Glycine max*	Accepted	C1=CC(=CC=C1C2=COC3 =CC(=CC(=C3C2=O)O)O)O
Luteolin	*Apium graveolens*	Accepted	C1=CC(=C(C=C1C2=CC(=O) C3=C(C=C(C=C3O2)O)O)O)O
Ellagic Acid	*Punica granatum*	Accepted	C1=C2C3=C(C(=C1O) O) OC (=O) C4=CC(=C(C(=C43) OC2=O) O) O
Rosmarinic Acid	*Rosmarinus officinalis*	Accepted	C1=CC(=C(C=C1CC(C(=O) O) OC(=O) C=CC2=CC(=C(C=C2) O) O) O) O

Table 3: Phytochemicals with their binding energy and amino acid residues.

Ligands	Binding energy (kcal/mol)	Amino acid residues
C=CCSS(=O)CC=C	-4.38	F42(B)CD2,R64(B)CG,E80(B)CB, D82(B)CB,K85(B)CB,D82(B)O, D82(B)N
COC1=C(C=CC(=C1)C=CC (=O)CC(=O)C=CC2=CC(=C (C=C2)O)OC)O	-6.38	V66(B) CG1,V66(B) CG2,T79(B) CG2,K85(B) CB, (B) CD2,I91(B) CD,R64(B) O,T79(B) O, T79(B) N,F42(B) N,D63(B) O, H72(B) ND1,W77(B) O,T79(B) ,R64(B) CA
COC1=C(C=CC(=C1)CC=C)O	-5.59	V40(B) CG1,V66(B) CG2,Y86(B) CD2,I91(B) CG1,D82(B) O,I81(B) N,D82(B) N,T79(B) O, E80(B) CA
CC1=CC(=C(C=C1)C(C)C)O	-5.91	F42(B) CD2,R64(B) CG,V66(B) CG2,I81(B) CB,D82(B) CB,Y86(B) CB,I91(B) CD,D82(B) O, D82(B) N,K84(B) O

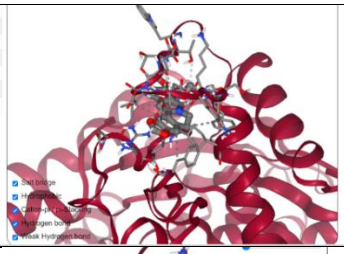
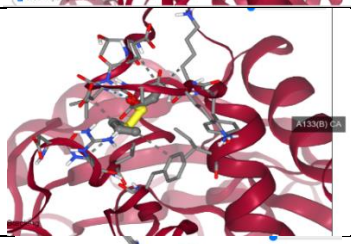
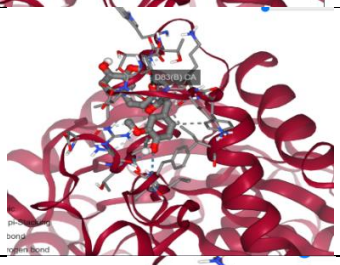
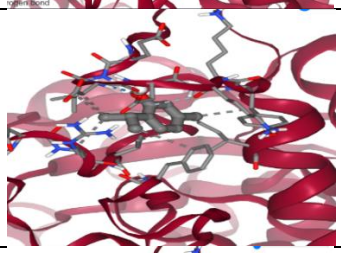
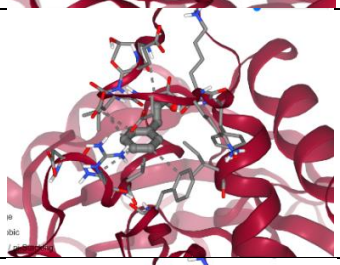
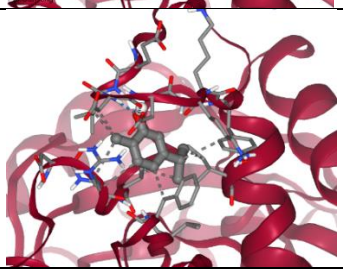
DOI: 10.69605/ijlbpr_14.5.2025.8

C1=CC=C(C=C1)C=CC=O	-5.25	F42(B) CD2,R64(B) CG,E80(B) CB,I81(B) CB,D82(B) CB,Y86(B) O,Y86(B) N
CC1=C(C=C(C=C1)C(C)C)O	-5.89	F42(B) CB,R64(B) CB,R64(B) CG,V66(B) CG2,I81(B) CB,D82(B) CB,Y86(B) CD2,I91(B) CG1, D82(B) O,D82(B) N
CC1CCC(C(C1)O)C(C)C	-6.28	F42(B) CB,V66(B) CG2,E80(B)CB,K85(B) CB, Y86(B) CD2,I91(B) CD,D82(B) O,D82(B) N
CC(C)C=CCCCCC(=O)NCC1 =CC(=C(C=C1)O)OC	-5.59	D367(B) CB, T369(B) CG2, P370(B) CG, I392(B) CG1, I392(B) CD, I452(B) CD, V458(B) CG2, I475(B) CG2, V458(B) O, I475(B) O, Q416(B) NE2, V458(B) N, I457(B) CA
COC1=C(C2=C[N+]3=C (C= C2C=C1) C4=CC5=C (C= C4CC3) OCO5) OC	-8.4	F42(B) C B, V66(B) CG2, T79(B) CG2, I81(B) CB, I81(B) CG1, Y86(B) CD2, T78(B) OG1,T79(B) O, T79(B) O, D82(B) O, Y86(B) O, H72(B) CE1
CC(=CCCC(C)(C=C)O)C	-5.49	V40(B) CB,V40(B) CG1,F42(B) CB,R64(B) CG,V66(B) CG2,I81(B) CD,D82(B) CB,I91(B) CG1, D82(B) O,D82(B) N
C1=CC(=CC=C1C=CC2=CC (=CC(=C2)O)O)O	-7.42	V40(B) CG1,F42(B) CB,V48(B) CG1,V66(B) CG2,Y86(B) CD2,I91(B) CG1,I91(B) CD,T79(B) O, R94(B) NH1,D82(B) N,R94(B) CD
CCCCCC(CC(=O)CCC1=CC (=C(C=C1)O)OC)O	-6.53	F42(B) CB,V66(B) CG1,V66(B) CG2,Y86(B) CD2,I91(B) CD,H72(B) NE2,D82(B) O,Y86(B) O,Y86(B) N,D82(B) N,H72(B) ND1,T78(B) CA
CC1=CCC(CC1)(C(C)C)O	-6.36	F42(B) CB,R64(B) CG,V66(B) CG2,E80(B) CB,I81(B) CB,K85(B) CB,I91(B) CD,D82(B) O,D82(B) N
C=CCC1=CC2=C(C=C1)OCO2	-6.14	F42(B) CD2,R64(B) CG,I81(B) CB,D82(B) CB,D83(B) CB,Y86(B) CD2,Y86(B) N,I81(B) N, K84(B) O,K85(B) CA,E80(B) CA
CC1=CCC2CC1C2(C)C	-5.8	F42(B) CD2,R64(B) CB,R64(B) CG,V66(B) CG2,E80(B) CB,I81(B) CB,D82(B) CB
C1=CC (=CC=C1C2=COC3= CC(=CC(=C3C2=O) O) O) O	-7.83	F42(B) CB,F42(B) CD2,R64(B) CB,V66(B) CG2,F42(B) O,T78(B) OG1,Y86(B) O,Y86(B) N,R64(B) NH1,T78(B) OG1,T79(B) O,K84(B) O, K85(B) CA,R64(B) CD
C1=CC(=C(C=C1C2=CC(=O) C3 =C(C=C(C=C3O2) O) O) O) O	-8.04	F42(B) CB,V48(B) CG1,Y86(B) CD2,I91(B) CG1,I91(B) CD,T79(B) O,D82(B) O,D82(B) O,Y86(B) O, R94(B) NH1,D82(B) N,R94(B) CD,I91(B) CA,R94(B) CD
C1=C2C3=C(C(=C1O) O) OC(=O) C4=CC(=C(C(=C43) OC2=O) O) O	-7.62	L153(B) CD2,V188(B) CB,T149(B) OG1,D158(B) OD1,G186(B) O,T149(B) OG1.V188(B) N,N146(B) N,T149(B)

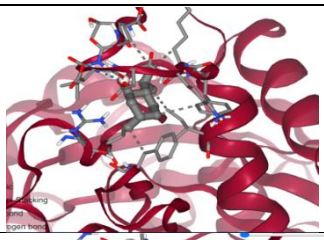
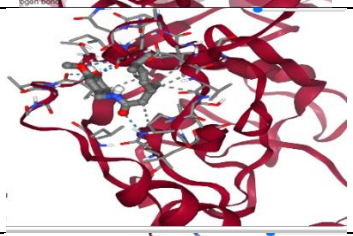
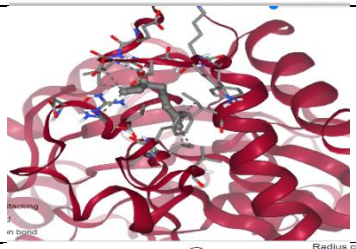
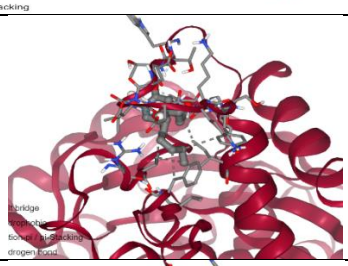
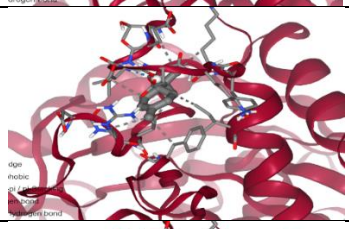
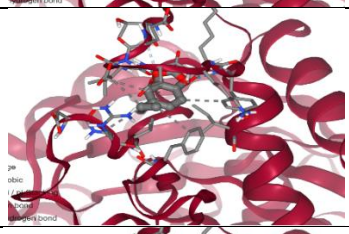
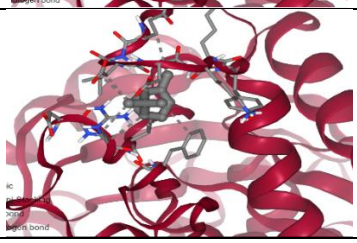
DOI: 10.69605/ijlbpr_14.5.2025.8

		OG1,Q352(BNE2,Q352(B) OE1,V187(B) CA
C1=CC(=C(C=C1CC(C(=O) O) OC(=O) C=CC2=CC(=C(C=C2) O) O) O) O	-5.42	R143(B) NE,V145(B) CG1,V188(B) CB,V355(B) CG1,T149(B) OG1,D158(B) OD1,D158(B) OD1,G186(B) O,V188(B) O,R143(B) NH1

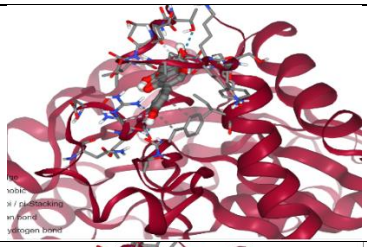
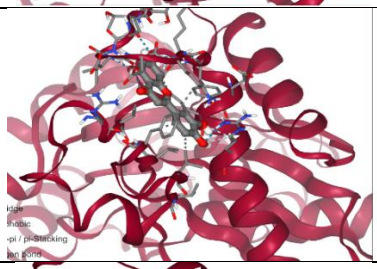
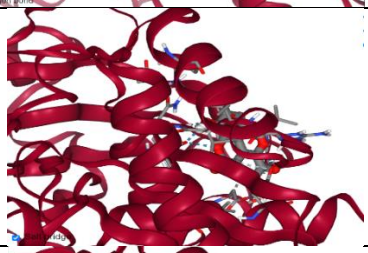
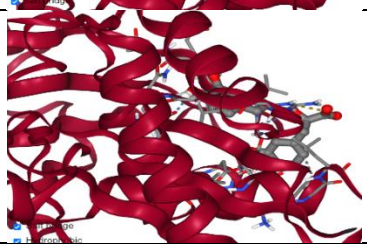
Table 4. The spatial molecular design of the in silico generated molecules

S. no.	Molecules	Molecular structure
1.	Berberine (-8.4)	
2.	Allicin (-4.38)	
3.	Curcumin (-6.38)	
4.	Thymol (-5.91)	
5.	Cinnamaldehyde (-5.25)	
6.	Carvacrol (-5.89)	

DOI: 10.69605/ijlbpr_14.5.2025.8

7.	Menthol (-6.28)	
8.	Capsaicin (-5.59)	
9.	Linalool (-5.49)	
10.	Resveratrol (-7.42)	
11.	Gingerol (-6.53)	
12.	Terpinen-4-ol (-6.36)	
13.	Safrole (-6.14)	
14.	Alpha-pinene (-5.8)	

DOI: 10.69605/ijlbpr_14.5.2025.8

15.	Genistein (-7.83)	
16.	Luteolin (-8.04)	
17.	Ellagic Acid (-7.62)	
18.	Rosmarinic Acid (-5.42)	

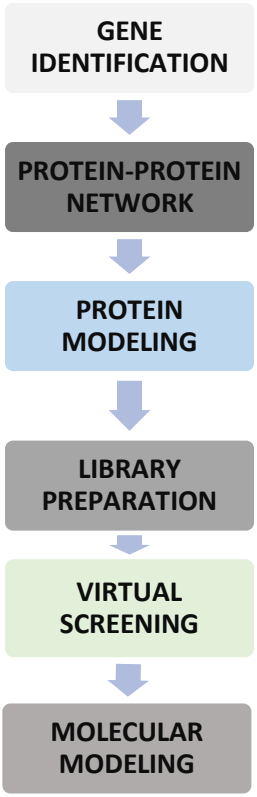


Figure 1. The steps involved in designing of phytochemicals

DOI: 10.69605/ijlbpr_14.5.2025.8

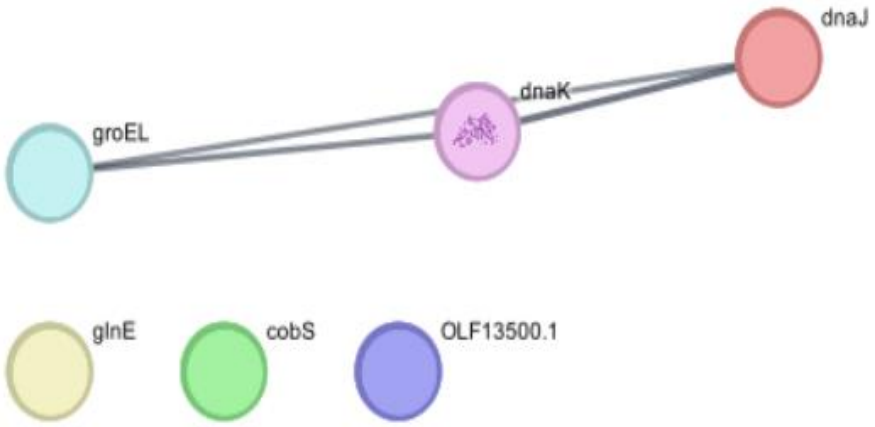


Figure 2. Protein – Protein Network

DISCUSSION

The rise in the incidence of fungal infections and evolution of new fungal strains is a global phenomenon at the helm of creating havoc. The already critical situation in exacerbated by the mounting antifungal resistance to commercially available antifungals. Therefore, there is a need to investigate new treatment options for fungal diseases. The intrigue in exploring the phyto-therapeutics in conjunction with the advent of in silico designing can give us a direction towards an environment friendly antifungal alternative. Ladyfinger is susceptible to several fungal diseases that impact its yield and quality (Table 1). Since these diseases reduce photosynthesis, they result in defoliation, vascular wilting, stem rot and fruit destruction, which causes severe loss.[3,4,5] As sustainable substitutes for synthetic fungicides, natural phytochemicals have been the subject of research into a variety of antifungal medicines for the treatment of various illnesses.[2]

In this study berberine was found to be the most effective antifungal phytochemical that can suppress fungal infections of okra. Through the disruption of fungal cell membranes, inhibition of enzymatic pathways, and interference with fungal DNA replication, berberine, an isoquinoline alkaloid, has potent antifungal effects. It has significant binding affinity to important fungal enzymes involved in pathogenicity, berberine was chosen as the most effective chemical based on molecular docking studies Its efficacy in animal infections have already been proven in previous studies.[6,7] In comparison to other plant-derived chemicals including flavonoids, tannins, and essential oils, berberine was found to be particularly efficient in regulating the development of *Fusarium oxysporum, Cercospora abelmoschi, Macrophomina phaseolina,* and *Podosphaera xanthii*. Due to its broad-spectrum antifungal properties, berberine is a possible treatment option for fungal illnesses in okra farming. The findings of this study are different from those of earlier research for a number of reasons. Firstly, although many earlier research relied on ethanol-based extractions which may have changed the composition of active chemicals. However, our work applied an aqueous extraction approach, which improved the bioavailability of berberine. Secondly, geographical variation plays a crucial role, as the phytochemical content in plants varies based on soil composition and climatic conditions, influencing their antifungal efficacy. Thirdly, this study used high concentration of berberine than previous studies, which resulted in better antifungal effects.[5,6,7] Also, this study assessed berberine's effectiveness against a wider variety of infections, offering a more thorough evaluation of its potential than earlier research that mostly examined particular fungal species.

The findings of our study showed "dnaK" gene has a significant role to play in okra infections. The discovery of the Powdery Mildew gene in *Podosphaera xanthii* represent a new approach also marks a new development that improves understanding of pathogenesis and consequently help in prevention and treatment of such infections. dnaK is a 70 kDa chaperone which prevents protein aggregation and assist the refolding of impaired proteins.[8] The integration of gene identification, protein-protein interaction, protein modelling, virtual screening and at last molecular docking techniques offered more precise and effective approach than conventional antifungal screenings. Further molecular-level evidence showed that berberine inhibits certain fungal proteins, a feature that hasn't been well studied in previous studies. This knowledge can be further researched upon to decode the of the connections between bacteria and fungi in okra diseases.

There are a few roadblocks that need to be taken care of while using phytochemicals. One of the main challenges in using phytochemicals as antifungal agents is their stability and correct formulation for field application. Many phytochemicals are volatile and can degrade quickly under field conditions. Developing stable formulations that ensure sustained release and efficacy is crucial. Like synthetic fungicides, there is a risk of pathogens developing resistance to phytochemicals.[2,5] Rotating different phytochemicals and using them in combination with

DOI: 10.69605/ijlbpr_14.5.2025.8

other control measures can help manage resistance development. Furthermore, like any new drug phytochemicals must undergo regulatory approval to ensure their safety and efficacy. Establishing standardized guidelines for their use and monitoring their impact on the environment and non-target organisms is essential.

Although the in-silico studies are the stepping stone for research, field trials are essential to validate the laboratory findings and determine the practical applicability of phytochemicals. Previous studies have proven that such phytochemicals discovered through molecular studies have been found to be effective in field studies too, for example neem oil applications reduces the incidence of anthracnose in okra fields, and clove oil can control powdery mildew effectively.[3,9,10] Phytochemicals can be integrated into pest management programs to reduce reliance on synthetic fungicides. Combining phytochemicals with cultural practices, resistant varieties, and biological control agents can enhance disease control while minimizing environmental impact. This study illustrates the novel use of molecular modelling and analytics to pinpoint the okra-resistant gene. Through the use of network analysis, 3D protein structure modelling, literature research, virtual screening of phytochemicals, and molecular docking investigations more such molecules can be repurposed for organic treatment options unburdening the already dry pipeline of antimicrobial agents. Continued research is needed to identify new phytochemicals with antifungal properties and understand their modes of action. Advances in biotechnology and genomics can aid in the discovery of novel compounds and the development of improved formulations.

CONCLUSION

This study gives insight on designing strategies for phytochemicals which can be used in broad spectrum of activities. Our results emphasized the role of dnaK gene in pathogenesis of fungal infections effecting okra and its correlation to antifungal activity of various phytochemicals. Berberine was found to be the most potent agent which is derived from *Hydrastic canadensis*. Our findings suggest the possibility of an alternative disease management strategy to control fungal diseases of okra. However, further research and validation are required to enhance the efficacy and stability of such phytochemicals for use in field use. This is a new avenue for scientific community to work upon and discover viable plant-based options for disease control.

REFERENCES

1. Elkhalifa AEO, Alshammari E, Adnan M, Alcantara JC, Awadelkareem AM, Eltoum NE et al. Okra (*Abelmoschus Esculentus*) as a Potential Dietary Medicine with Nutraceutical Importance for Sustainable Health Applications. Molecules. 2021;26(3):696. doi: 10.3390/molecules26030696.
2. Deresa EM. Diriba TF. Phytochemicals as alternative fungicides for controlling plant diseases: A comprehensive review of their efficacy, commercial representatives, advantages, challenges for adoption, and possible solutions. Heliyon. 2023;9(3):e13810. doi: 10.1016/j.heliyon.2023.e13810.
3. Khare CP, Nema S, Srivastava JN, Yadav VK, Sharma ND. (2015). Fungal Diseases of Okra (*Abelmoschus esculentus* L.) and Their Integrated Management (IDM). In: Awasthi, L.P. (eds) Recent Advances in the Diagnosis and Management of Plant Diseases. Springer, New Delhi. https://doi.org/10.1007/978-81-322-2571-3_8
4. Ashwini R, Amaresh YS, Yenjerappa ST, Kulkarni S, Aswathanarayana DS. Studies on Symptomatology, Morphological and Molecular Characterisiation of Erysiphe Cichoracearum Causing Powdery Mildew of Okra. International Journal of Environment and Climate Change. 2023;13(10):2921-28. https://doi.org/10.9734/ijecc/2023/v13i102958.
5. Malik AA, Ahmed N, Babita, Chauhan H, Gupta P. Plant Extracts in Post-Harvest Disease Management of Fruits and Vegetables-A Review. J Food Process Technol. 2016;7:592. doi:10.4172/2157-7110.1000592
6. Zhang CW, Huang DY, Rajoka MSR, Wu Y, He ZD, Ye L et al. The Antifungal Effects of Berberine and Its Proposed Mechanism of Action Through CYP51 Inhibition, as Predicted by Molecular Docking and Binding Analysis. Molecules. 2024;29(21):5079. doi: 10.3390/molecules29215079.
7. da Silva AR, de Andrade Neto JB, da Silva CR, Campos Rde S, Costa Silva RA, Freitas DD et al. Berberine Antifungal Activity in Fluconazole-Resistant Pathogenic Yeasts: Action Mechanism Evaluated by Flow Cytometry and Biofilm Growth Inhibition in Candida spp. Antimicrob Agents Chemother. 2016;60(6):3551-7. doi: 10.1128/AAC.01846-15.
8. Stepkowski T, Czaplińska M, Miedzinska K, Moulin L. The variable part of the dnaK gene as an alternative marker for phylogenetic studies of rhizobia and related alpha Proteobacteria. Syst Appl Microbiol. 2003;26(4):483-94. doi: 10.1078/072320203770865765.
9. Kumar V, Chaudhary VP, Kumar D, Kumar A, Sagar S, Chaudhary S. Efficacy of botanicals and fungicides against Rhizoctonia solani inciting sheath blight disease on Rice (Oryza sativa L.). Journal of Applied and Natural Science. 2017;9(4),1916-1920. https://doi.org/10.31018/jans.v9i4.1463
10. Abdel-Kader M, El-Mougy N, El-Gammal NG, Abd-El-Kareem F, Abd-Alla MA. Laboratory Evaluation of Some Chemicals Affecting Pathogenic Fungal Growth. Journal of Applied Sciences Research. 2012;8(1): 523-530.