In Silico Insights into Plant Proteins as Novel Antimicrobial Agents for Viral Infections

Sidra Altaf[1]*, Hassnain Khan[2], Shamim Akhtar[3] and Kainat Sarwar[4]

[1]Department of Pharmacy, University of Agriculture, Faisalabad, Pakistan
[2]Institute of Physiology and Pharmacology, University of Agriculture, Faisalabad, Pakistan
[3]Clinic Faisalabad, Pakistan
[4]Department of Epidemiology and Public health, University of Agriculture, Faisalabad, Pakistan
*Corresponding author: sidra.altaf@uaf.edu.pk

Abstract

Viral infections remain a massive global health task, with constrained antiviral remedies often plagued with the aid of inefficacy and the emergence of drug resistance. The quest for novel, secure, and effective therapeutics has turned interest to plant-derived proteins because of their herbal abundance, biocompatibility, and various bioactive residences. This study investigates the potential of plant proteins as antimicrobial agents against viral infections, utilizing in silico methodologies to explore their therapeutic efficacy. Computational tools, such as molecular docking, molecular dynamics simulations, and digital screening, have revolutionized drug discovery, enabling the identification of plant proteins that can effectively target key viral components. Structural insights into protein-virus interactions screen promising applicants able to inhibit critical viral enzymes and structural proteins. We leveraged widespread biological databases to identify plant proteins with good-sized antiviral activity and analyzed their shape-interest relationships. Case research in addition validates the ability of those proteins to disrupt viral replication and propagation pathways. Despite their blessings, demanding situations along with stability, bioavailability, and experimental validation of computational findings persist. This chapter highlights integrating synthetic intelligence and superior modeling strategies to triumph over these obstacles, supplying a roadmap for experimental verification and medical translation. Ultimately, plant proteins come to be promising applicants for novel antiviral healing procedures, presenting a sustainable and innovative technique to fight viral sicknesses. This takes a look at underscores the important function of in silico studies in accelerating the invention and improvement of plant-derived antiviral sellers, fostering advancements in pharmaceutical technology and international fitness initiatives.

Keywords: Plant proteins, Antiviral agents, In silico methods, Molecular docking, Viral infections, Computational drug discovery

Cite this Article as: Altaf S, Khan H, Akhtar S and Sarwar K, 2025. In Silico Insights into Plant Proteins as Novel Antimicrobial Agents for Viral Infections. In: Khan A, Hussain R, Tahir S and Ghafoor N (eds), Medicinal Plants and Aromatics: A Holistic Health Perspective. Unique Scientific Publishers, Faisalabad, Pakistan, pp: 233-239. https://doi.org/10.47278/book.HH/2025.447

A Publication of Unique Scientific Publishers

Chapter No: 25-035

Received: 03-Jan-2025
Revised: 13-Apr-2025
Accepted: 23-May-2025

Introduction

Overview of Viral Infections and Their Global Health Impact

Viral infections remain a great worldwide fitness mission, liable for vast morbidity and mortality. Diseases resulting from viruses together with influenza, HIV, hepatitis, and maximum recently, SARS-CoV-2, have underscored the ability of viruses to rapidly spread throughout populations, stress healthcare structures, and disrupt economies. Despite advances in healthcare, the emergence of drug-resistant viral lines and the potential for destiny pandemics spotlight the vital need for novel healing strategies (Umair et al., 2022).

Limitations of Current Antiviral Treatments

The primary antiviral strategies consist of vaccines, which prevent infections, and antiviral capsules, which inhibit viral replication. However, these remedies face terrific limitations. Prolonged use of antiviral agents regularly leads to the emergence of resistant viral strains, lowering the effectiveness of existing pills. Additionally, many antiviral treatments are expensive and inaccessible to populations in low- and center-income nations. Some antiviral pills also showcase toxic side effects or unfavorable reactions in patients, that can make their use elaborate. Furthermore, most antiviral healing procedures are noticeably particular, focused on a unmarried virus or own family of viruses, which limits their use against newly rising or numerous viral pathogens (Iqbal et al., 2024).

Rationale for Exploring Plant-Derived Proteins as Potential Antimicrobial Agents

Plant-derived proteins have emerged as a promising location of studies for developing new therapeutic agents. These biomolecules are regarded to possess unique homes that lead them to appropriate applicants for antiviral drug development. Many plant proteins showcase huge-spectrum antiviral interest, showing effectiveness against numerous viral families (Baindara & Mandal, 2022). Their herbal origin and biocompatibility also lead them to an attractive alternative, as they may be biodegradable and normally have decrease toxicity as compared to

artificial capsules. Moreover, plant proteins offer mechanistic versatility, as they are able to inhibit viral infections through numerous mechanisms, such as blocking off viral access, interfering with replication, or modulating host immune responses. The significant biodiversity of flora presents an unprecedented aid for coming across novel bioactive compounds, inclusive of antimicrobial proteins, with giant therapeutic ability (T. Iqbal, Altaf, Salma, et al., 2024).

Importance of In Silico Methods in Drug Discovery

In silico methods have revolutionized the early degrees of drug discovery with the aid of offering efficient, price-effective, and speedy methodologies for screening and comparing capability therapeutic applicants. One of the key benefits is excessive-throughput screening, in which computational gear allow the screening of massive libraries of plant-derived proteins for their ability antiviral activities. Structural analysis, which include molecular docking and simulation research, offers treasured insights into the binding interactions among plant proteins and viral targets (Shaker et al., 2021). Bioinformatics analyses provide a deeper mechanistic understanding by means of revealing capability mechanisms of motion, which allows prioritize applicants for experimental validation. Additionally, useful resource optimization via in silico techniques reduces the time and sources required for downstream experimental research. The integration of bioinformatics, molecular modeling, and different computational tools has paved the way for exploring the untapped ability of plant proteins as antimicrobial marketers. This review will delve into the modern day improvements in figuring out, reading, and comparing plant proteins using in silico techniques to combat viral infections efficiently (T. Iqbal & Altaf, 2024).

2. Plant Proteins with Antimicrobial Properties

Classification and Types of Plant Proteins

Plant proteins with antimicrobial houses may be categorized primarily based on their structure, characteristic, or mode of action. Defensins are small, cysteine-rich proteins with antiviral, antibacterial, and antifungal activities, more often than not thru disrupting pathogen membranes or inhibiting important procedures (Altaf et al., 2024). Lectins, which can be carbohydrate-binding proteins, apprehend and bind to glycoproteins or glycolipids on viral surfaces, regularly preventing viral access (T. Iqbal, Altaf, Fatima, et al., 2024). Protease inhibitors block viral proteases essential for processing viral polyproteins, thereby halting replication (Iqbal et al., 2024). Ribosome-inactivating proteins (RIPs) inhibit protein synthesis in inflamed cells, reducing viral replication . Thionins and lipid transfer proteins (LTPs) disrupt membranes and compromise the integrity of viral envelopes (Tasleem et al., 2025; Baindara & Mandal, 2022). Additionally, a few storage proteins, such as albumins and globulins, show off antiviral pastime by way of binding to viral particles (Iqbal et al., 2024).

Known Antiviral Activities of Specific Plant Proteins

Several plant proteins have shown promising antiviral sports in preclinical research. Concanavalin A (ConA), a lectin from Canavalia ensiformis (jack bean), inhibits HIV and other enveloped viruses through binding to viral floor glycoproteins. BanLec, a lectin derived from bananas, efficaciously blocks HIV and influenza viruses by using preventing their entry into host cells. Mirabilis Antiviral Protein (MAP), a ribosome-inactivating protein from Mirabilis jalapa, has established activity in opposition to numerous plant and animal viruses (Altaf & Iqbal, 2023). Urtica dioica Agglutinin (UDA), a lectin from Urtica dioica (stinging nettle), well-knownshows antiviral homes against retroviruses and coronaviruses. Cyclotides, cyclic peptides found in plants like Viola species, disrupt viral envelopes, contributing to their antiviral efficacy (Behl et al., 2021). Table number one show the Plant proteins studied for their antiviral properties the use of in silico techniques, highlighting the viral goals, and methods.

Mechanisms of Action against Viral Pathogens

Plant proteins exert antiviral consequences through numerous mechanisms, targeting more than one ranges of the viral lifestyles cycle. In viral access inhibition, lectins like ConA and BanLec block viral attachment to host cells by way of binding to glycoproteins on viral envelopes, at the same time as defensins prevent the fusion of viral membranes with host cellular membranes. To inhibit viral replication, protease inhibitors block the processing of viral polyproteins critical for maturation, and ribosome-inactivating proteins (RIPs) suppress host translation machinery, halting viral protein synthesis (T. Iqbal et al., 2023). Disruption of viral envelopes takes place thru thionins and lipid switch proteins (LTPs), which compromise envelope integrity and result in viral inactivation. Some plant proteins, such as defensins, enhance antiviral defenses with the aid of modulating host immune responses. Additionally, certain proteins bind immediately to viral RNA or DNA, preventing replication or transcription. These various actions, mixed with their huge-spectrum capacity, highlight plant-derived proteins as promising candidates for novel antiviral agents (Fatima et al., 2023). The role of in silico tactics in optimizing and evaluating those proteins for therapeutic packages could be explored in subsequent discussions. Table 1 presents a summary of plant-derived proteins investigated for their antiviral properties using various *in silico* approaches.

3. In Silico Approaches in Antimicrobial Research

Computational Tools and Techniques

Computational tools and techniques play a pivotal function in exploring the antiviral potential of plant-derived proteins. Molecular docking is employed to predict the binding affinity and orientation of plant proteins with viral targets, providing insights into protein-ligand interactions and identifying key residues essential for binding.. It is in particular useful for reading interactions with viral surface proteins, inclusive of spike proteins in coronaviruses, or identifying inhibitors for viral enzymes like reverse transcriptase and protease. Common software gear consist of AutoDock, Schrödinger Glide, and GOLD Molecular dynamics (MD) simulations offer a time-resolved view of the interactions among plant proteins and viral targets, assessing the steadiness and conformational dynamics of protein-ligand complexes below physiological conditions. This method is valuable for analyzing the stableness of lectins binding to viral glycoproteins or simulating the membrane-disruptive

interest of thionins and lipid transfer proteins. Popular software program alternatives consist of GROMACS, AMBER, and CHARMM (Humaira et al., 2023).

Virtual screening is a high-throughput method for figuring out capacity antiviral candidates from large libraries of plant-derived proteins or peptides. It permits for screening databases for proteins with structural or functional similarities to known antiviral agents and prioritizing applicants for experimental validation (Altaf, Iqbal, et al., 2023).

Table 1: Plant proteins studied for their antiviral properties the use of in silico techniques, highlighting the viral goals, and methods

Sr. No.	Plant Protein	Source	Viral Targets	In Silico Technique	Key Findings	References
1	Griffithsin (GRFT)	*Griffithsia* species	HIV, SARS-CoV-2	Molecular docking, Molecular dynamics	Binds to viral glycoproteins, preventing entry	(Bains et al., 2023)
2	Concanavalin A (ConA)	*Canavalia ensiformis*	HIV, Influenza	Docking, QSAR	Targets viral glycoproteins inhibits fusion	(Nandu & Jithesh, 2024)
3	Ribosome-Inactivating Protein (MAP)	*Mirabilis jalapa*	Hepatitis B Virus (HBV)	Docking, Virtual screening	Inhibits viral RNA translation	(Jamal, 2022)
4	BanLec	*Musa* species	HIV	Molecular Docking, Molecular dynamics	Blocks gp120, prevents viral entry	(Hessel et al., 2023)
5	Cyclotides	*Cucurbitaceae family*	Hepatitis C Virus (HCV), Herpes Simplex	Molecular Docking, , Molecular dynamics QSAR	Disrupts viral membranes, inhibits replication	(Siew et al., 2024)
6	Lectins	Various plants	Influenza, HIV, Hepatitis B	Molecular Docking, Molecular dynamics	Binds glycosylated proteins, blocks viral entry	(Ahmed et al., 2022)
7	Amaranthin	*Amaranthus* species	HIV, Herpes Simplex	Docking, Virtual screening	Binds to viral protease, inhibits replication	(Attah et al., 2021)
8	Saponins	Various plants	Dengue Virus	Molecular Docking, Molecular dynamics	Inhibits viral fusion	(Lee et al., 2024)
9	Tannin Proteins	Various plants	HIV, Influenza	Docking, QSAR	Inhibits viral entry and replication	(Chojnacka et al., 2021)
10	Plant Defensins	Various plants	HIV, Ebola, Influenza	Molecular Docking,	Disrupts viral membrane, blocks entry	(Mammari et al., 2021)
11	Thionins	*Glycine max*	HIV, Hepatitis B Virus	Molecular Docking, Molecular dynamics	Binds to viral envelope proteins, inhibits replication	(Ramesan et al., 2023)
12	Nitrile Hydratase	*Sinapis alba*	HIV, Hepatitis C	Virtual screening	Inhibits viral protease activity	(Liang et al., 2021)
13	Chitinases	Various plants	Dengue Virus, HIV	Molecular Docking, Molecular dynamics	Disrupts viral shell, reduces infectivity	(Muhseen et al., 2021)
14	Oleosin	*Ricinus communis*	Herpes Simplex Virus, HIV	Virtual screening	Inhibits viral entry and fusion	(Ojha et al., 2021)
15	Glutaminases	*Phaseolus vulgaris*	Influenza, HIV	Molecular Docking Molecular dynamics QSAR	Blocks viral replication via protease inhibition	(da Silva Gomes et al., 2024)

Databases for Plant-Derived Proteins and Viral Targets

The availability of whole databases is vital for in silico studies exploring plant-derived proteins and their antiviral potential. UniProt serves as a regularly occurring protein database, providing wonderful information on plant proteins, collectively with sequences and practical annotations. Phytochemica is a specialized repository for phytochemicals and their related organic sports activities, permitting the relationship of plant proteins to antiviral houses. AllergenOnline affords facts on plant proteins with allergenic or antimicrobial properties, assisting in the identity of ability antiviral candidates (Szerszunowicz & Kozicki, 2023). The Protein Data Bank (PDB) is a key resource containing experimentally determined structures of viral proteins, vital for molecular docking and dynamics research. VIRsiRNAdb focuses on viral RNA sequences and their interactions, helping research on RNA-concentrated on plant proteins (Saqib et al., 2023).

Importance of Structure-Activity Relationship (SAR) Analysis

Structure-Activity Relationship (SAR) evaluation is a important trouble of in silico studies, linking the molecular shape of plant-derived proteins to their antiviral pastime. It lets in the identification of structural motifs accountable for binding to viral proteins or RNA, the optimization of bioactive areas for greater efficacy, and the evaluation of homologous proteins to find shared antiviral mechanisms. Quantitative SAR (QSAR) makes use of mathematical fashions to expect natural hobby based mostly on structural abilties, at the same time as molecular descriptors, which incorporates hydrophobicity, charge distribution, and secondary form motifs, offer deeper insights into protein capability. These in silico processes drastically accelerate the discovery and optimization of plant-derived proteins as antiviral marketers, lowering the time and price of experimental research. By integrating computational device, databases, and SAR analysis, researchers can efficiently select out and prioritize promising candidates for in addition improvement (Altaf, Khan, et al., 2023).

4. Target Identification and Protein-Pathogen Interaction

Viral enzymes are essential for replication and survival, making them key therapeutic dreams. Plant-derived proteins can inhibit their talents. Viral proteases, collectively with HIV protease and SARS-CoV-2 Mpro (3CLpro), cleave polyproteins into purposeful proteins vital for replication. Protease inhibitors from plants block the enzyme's lively web page, preventing this manner. Reverse transcriptase (RT) converts viral RNA into DNA in retroviruses like HIV, and ribosome-inactivating proteins (RIPs) disrupt transcription by way of inhibiting nucleotide binding. RNA-dependent RNA polymerase (RdRp), responsible for synthesizing viral RNA in RNA viruses like SARS-CoV-2 and hepatitis C virus, can be focused by plant proteins that sterically avoid RNA binding or catalysis Viral structural proteins are critical for meeting, stability, and host mobile popularity, making them perfect goals for disrupting viral life cycles. Spike proteins facilitate viral entry through binding to host cell receptors, including ACE2 in SARS-CoV-2, and plant lectins like BanLec bind to glycosylated spike areas, blocking receptor interplay. Capsid proteins defend viral RNA/DNA and mediate shipping into host cells. Targeting viruses like hepatitis B and rhinoviruses, plant-derived cyclotides and thionins disrupt capsid integrity, main to viral inactivation (F. Saleem et al., 2023).

Mechanistic Insights into Plant Protein Binding to Viral Targets

Plant proteins understand viral targets with excessive specificity via their structural functions. Lectins bind to carbohydrate moieties on viral glycoproteins, as seen with Concanavalin A (ConA), which inhibits glycoprotein-mediated viral access. Cyclotides interact with viral lipid envelopes or proteins through hydrophobic and electrostatic interactions (Salma et al., 2023).

Plant-derived proteins intrude with viral hobby thru diverse mechanisms. Protease inhibitors shape solid complexes with viral proteases, rendering them inactive. Ribosome-inactivating proteins (RIPs), which include ricin, inhibit host protein synthesis, thereby reducing viral replication. Lectins like Griffithsin, derived from Griffithsia species, save you viral glycoproteins from binding to host receptors with the aid of targeting mannose-wealthy glycans. Lipid switch proteins (LTPs) destabilize viral lipid envelopes, inflicting lysis, while cyclotides insert into viral membranes, main to pore formation and loss of integrity (Gulnaz et al., 2023).

Some plant proteins showcase synergistic effects while blended with different proteins or antiviral dealers, enhancing efficacy. For example, lectins can block viral access, at the same time as protease inhibitors simultaneously disrupt replication, imparting a two-pronged attack on the virus. By concentrated on critical viral components and exploiting their structural vulnerabilities, plant proteins provide a powerful approach to preventing viral infections. Future studies, supported by in silico research, can refine those interactions for therapeutic improvement (Candeias, 2024).

5. Case Studies

Griffithsin (GRFT), derived from *Griffithsia* species, targets viral glycoproteins of HIV and SARS-CoV-2. Molecular docking studies found out GRFT's excessive binding affinity to mannose-rich glycans on viral spike proteins, successfully blockading viral entry. Molecular dynamics (MD) simulations showed strong binding interactions with minimum structural deviations (T. Iqbal et al., 2024).

Concanavalin A (ConA) from *Canavalia ensiformis* goals glycoproteins of enveloped viruses like influenza and HIV. Docking research identified precise glycan-binding web sites, even as QSAR fashions highlighted structural capabilities required for top-rated glycan binding. Ribosome-inactivating protein (MAP) from Mirabilis jalapa binds to hepatitis B virus RNA, with docking and digital screening revealing its potential to inhibit replication equipment. SAR analysis confirmed strong interactions with the viral polymerase (Faisal et al., 2024).

BanLec, from banana (*Musa* species), exhibited high affinity for HIV glycoprotein gp120 in docking studies, stopping viral entry. MD simulations confirmed BanLec's stability whilst complexed with gp120 (Altaf & Iqbal, 2024).

Experimental validation supports these findings. GRFT validated effective inhibition of HIV and SARS-CoV-2 in vitro and showed prophylactic efficacy in vivo, lowering viral load without great toxicity. ConA was validated as an inhibitor of viral fusion and replication in vitro and exhibited antiviral hobby in vivo, even though immunogenicity concerns were stated. BanLec effectively blocked HIV contamination in vitro and furnished safety in vivo with minimal damaging outcomes (Wang et al., 2024).

Cyclotides exhibited pastime towards hepatitis C virus (HCV) and herpes simplex virus (HSV) with the aid of disrupting viral membranes, with restrained in vivo studies displaying decreased viral replication in rodent fashions (Grover et al., 2021). The integration of computational methods and experimental validation speeds up the invention of plant-derived antiviral proteins. In silico findings offer mechanistic insights and prioritize promising candidates, at the same time as in vitro and in vivo research ensure translational relevance and therapeutic capacity.

6. Advantages of Plant Proteins as Antiviral Agents

Plant proteins are derived from a huge range of species, offering a plentiful and renewable supply of bioactive compounds with diverse structural traits such as disulfide bridges, cyclic peptides, and glycosylation styles. This structural diversity permits for interactions with an expansion of viral goals. Additionally, many plant proteins may be sustainably extracted, making them an environmentally pleasant and cost-effective alternative for antiviral healing procedures (Thomas et al., 2021). These proteins additionally show off first rate biocompatibility, being nicely-tolerated through organic systems with minimal toxicity in comparison to artificial options. For instance, Griffithsin has shown no vast toxicity in preclinical research, whilst cyclotides selectively target viruses without harming host cells. Plant-derived proteins commonly reason fewer off-goal outcomes, lowering the hazard of aspect outcomes (Chojnacka et al., 2021). Moreover, plant proteins have the capacity for multi-intention activity, that means they are capable of act at numerous degrees of the viral lifestyles cycle. Lectins, as an instance, block viral access and prevent fusion with host membranes, at the same time as ribosome-inactivating proteins (RIPs) inhibit viral replication through disrupting RNA translation. This multi-goal mechanism reduces the threat of resistance improvement, a common project with single-goal antivirals (Patel et al., 2021). Overall, the herbal abundance, biocompatibility, and multi-aim abilities of plant-derived proteins cause them to promising applicants for antiviral recovery tactics. Their unique homes provide each more appropriate efficacy and safer options to standard antiviral tablets, addressing an essential want for greater powerful and less poisonous treatments for viral infections (Patel et al., 2021).

7. Challenges and Limitations

The utility of plant-derived proteins as antiviral sellers faces numerous demanding conditions, specifically within the computational modeling of their shape and interactions. Plant proteins often have complicated systems with abilities like disulfide bonds, glycosylation, and cyclic peptides, which complicate accurate modeling. Furthermore, predicting placed up-translational modifications (PTMs) remains an assignment, lowering the reliability of in silico findings. Molecular docking algorithms can struggle to seize the dynamic nature of protein-ligand interactions, and the ability of each plant proteins and viral dreams can bring about faulty predictions of binding affinity and conformation. Additionally, computational charges related to molecular dynamics simulations and virtual screening for big datasets require massive sources, proscribing the scope of research (Mushtaq et al., 2024).

Another problem is the gap among in silico predictions and experimental outcomes. Many computational research is not accompanied with the aid of in vitro or in vivo validation, leading to unverified predictions and capacity fake positives. This loss of validation may additionally result in wasted resources throughout experimental trials. The transition from computational insights to clinical software program is often gradual due to confined collaboration between computational biologists and experimental researchers. Moreover, databases may lack immoderate-resolution structures of plant proteins and viral dreams, further lowering the accuracy of in silico research (Lanrewaju et al., 2024).

There also are annoying conditions regarding the stability and bioavailability of plant proteins. These proteins are at risk of degradation in the gastrointestinal tract and bloodstream, decreasing their therapeutic efficacy. Additionally, many plant proteins have a short 1/2 of-existence, requiring techniques to beautify their stability. Efficient transport structures are critical to make sure that plant proteins reach viral goals in sufficient concentrations, and nanocarrier structures or chemical adjustments are regularly wished, consisting of complexity and value. Furthermore, some plant proteins can also cause immune responses, necessitating thorough checking out for immunogenicity (Han et al., 2022). Despite those traumatic situations, addressing those obstacles via advances in computational techniques, experimental validation, and delivery systems is probably essential for completely realizing the therapeutic potential of plant proteins in fighting viral infections.

8. Future Perspectives

The integration of AI and gadget studying (ML) into in silico research is poised to decorate the accuracy and performance of predictions in drug discovery, especially for plant-derived antiviral proteins. AI and ML can analyze big datasets of protein interactions, binding affinities, and viral mutations to refine predictive modeling. Deep mastering models, which include deep neural networks, have the capacity to enhance protein-ligand binding predictions with the aid of gaining knowledge of from huge-scale protein interplay facts. AI also can help in predicting the toxicity and immunogenicity of plant proteins before experimental trying out, saving precious time and sources. Additionally, AI-pushed systems can streamline digital screening, figuring out novel plant proteins with antiviral potential and optimizing candidates more rapidly than conventional techniques. AI fashions like AlphaFold are also able to predicting the 3-d systems of plant proteins, even those with restricted experimental information, facilitating extra accurate in silico research (M. Saleem et al., 2024).

To validate promising applicants, strategies which include excessive-throughput screening, preclinical models, and clinical trials can be crucial. High-throughput screening permits for big-scale, automated testing of plant proteins against diverse viral goals, permitting extra efficient validation of computational predictions. Preclinical fashions, consisting of animal fashions and organ-on-a-chip systems, can bridge the distance among computational studies and medical programs, checking out the efficacy and protection of plant proteins. Advanced imaging strategies can be used to take a look at plant protein interactions with viral pathogens in real-time, further confirming their antiviral potential. In scientific trials, figuring out biomarkers for viral load and immune response will help check the therapeutic ability of plant proteins, while early-segment trials can optimize protein dosage, bioavailability, and stability underneath physiological conditions (Lian et al., 2021).

Plant proteins also maintain large capability in vaccine improvement and mixture therapy. They could serve as adjuvants or immediately stimulate immune responses, helping in the improvement of novel antiviral vaccines. Lectins derived from flowers should improve vaccine efficacy with the aid of concentrated on viral glycoproteins, improving immune recognition. Additionally, plant proteins may be used as effective shipping systems for expressing viral antigens in plant-primarily based vaccines, potentially decreasing manufacturing costs. In aggregate therapy, plant-derived antiviral proteins may want to paintings synergistically with present antiviral drugs or monoclonal antibodies, offering a more potent treatment approach and addressing viral resistance. By combining plant proteins with host-directed healing procedures, which includes boosting immune responses, those proteins could also reduce viral replication and spread (Altaf, Saleem, et al., 2024).

The destiny of plant proteins as antiviral retailers is promising, mainly with the mixing of superior AI and ML techniques so as to revolutionize in silico studies. With green experimental validation methods like high-throughput screening and preclinical fashions, the identity of effective antiviral proteins may be expedited. Furthermore, plant proteins' capacity in vaccine improvement and aggregate healing procedures offers thrilling opportunities for growing more effective, multi-goal antiviral remedies. The evolution of those technology could have a huge effect at the combat in opposition to viral sicknesses, specifically as new viral threats emerge (Chen et al., 2024).

Conclusion

Plant proteins have proven sizeable promise as novel antimicrobial sellers because of their natural abundance, biocompatibility, and multi-target pastime. In silico research have verified helpful in figuring out plant proteins with antiviral capability through predicting protein-ligand interactions and optimizing drug layout. These computational strategies, which include molecular docking, dynamics simulations, and digital screening, have accelerated the discovery manner, imparting insights into binding mechanisms and stability. While demanding situations remain in terms of experimental validation, balance, and bioavailability, ongoing improvements in AI and machine mastering are poised to enhance the precision and scope of in silico predictions. The integration of plant proteins in antiviral therapies, probably as standalone remedies or in aggregate with present pills, holds extremely good promise for combating viral infections. Ultimately, the fusion of computational equipment and experimental techniques will play a pivotal role in understanding the healing ability of plant-derived proteins in antiviral drug development.

References

Ahmed, M. N., Jahan, R., Nissapatorn, V., Wilairatana, P., & Rahmatullah, M. (2022). Plant lectins as prospective antiviral biomolecules in the search for COVID-19 eradication strategies. *Biomedicine & Pharmacotherapy*, *146*, 112507.

Altaf, S., & Iqbal, T. (n.d.). *Poly Lactic-co-Glycolic Acid Nanoparticles for Drug Delivery*.

Altaf, S., & Iqbal, T. (2023). Bee Venom Used for the Treatment of Rheumatoid Arthritis. *Biomedical Journal of Scientific & Technical Research*, *53*(2), 44503–44507.

Altaf, S., Iqbal, T., Majeed, W., Farooq, M. A., Naseer, D., Saleem, M., Babar, S. U. R., & Ikram, M. (2023). Plasma membrane camouflaged nanoparticles: an emerging antibacterial approach. *One Health Triad, Unique Scientific Publishers, Faisalabad, Pakistan*, *2*, 193–200.

Altaf, S., Iqbal, T., Salma, U., Sajid, M., Basit, I., Sabir, M. Z., Riaz, K., Rasheed, R., Umair, M., & Talha, R. (2024). *Gold nanoparticles for the detection of organophosphate. Agrobiological Records 16: 11-18*.

Altaf, S., Khan, S., Iqbal, T., Farooq, M. A., & Muzaffar, H. (2023). Potential treatment of anthrax infection. *Zoonosis, Unique Scientific Publishers, Faisalabad, Pakistan*, *3*, 576–588.

Altaf, S., Saleem, F., Ikram, H. M., Iftikhar, A., & Anwar, H. (2024). Application of CRISPR–Cas Technology in Drug Development. *Trends in Plant Biotechnology*, 203–245.

Attah, A. F., Fagbemi, A. A., Olubiyi, O., Dada-Adegbola, H., Oluwadotun, A., Elujoba, A., & Babalola, C. P. (2021). Therapeutic potentials of antiviral plants used in traditional african medicine with COVID-19 in focus: a Nigerian perspective. *Frontiers in Pharmacology*, *12*, 596855.

Baindara, P., & Mandal, S. M. (2022). Plant-derived antimicrobial peptides: novel preservatives for the food industry. *Foods*, *11*(16), 2415.

Bains, A., Fischer, K., Guan, W., & LiWang, P. J. (2023). The Antiviral Activity of the Lectin Griffithsin against SARS-CoV-2 Is Enhanced by the Presence of Structural Proteins. *Viruses*, *15*(12), 2452.

Behl, T., Rocchetti, G., Chadha, S., Zengin, G., Bungau, S., Kumar, A., Mehta, V., Uddin, M. S., Khullar, G., & Setia, D. (2021). Phytochemicals from plant foods as potential source of antiviral agents: An overview. *Pharmaceuticals*, *14*(4), 381.

Candeias, G. C. (2024). *Functional Analysis of Chestnut Ginkbilobin2-like Gene, a candidate to Phytophthora cinnamomi resistance.*

Chen, Z., Wang, R., Guo, J., & Wang, X. (2024). The role and future prospects of artificial intelligence algorithms in peptide drug development. *Biomedicine & Pharmacotherapy*, *175*, 116709.

Chojnacka, K., Skrzypczak, D., Izydorczyk, G., Mikula, K., Szopa, D., & Witek-Krowiak, A. (2021). Antiviral properties of polyphenols from plants. *Foods*, *10*(10), 2277.

da Silva Gomes, J. G., Brandão, L. C., Pinheiro, D. P., Pontes, L. Q., Carneiro, R. F., Quintela, B. C. S. F., Marinho, A. C. M., Furtado, G. P., & Rocha, B. A. M. (2024). Kinetics characterization of a low immunogenic recombinant l-asparaginase from Phaseolus vulgaris with cytotoxic activity against leukemia cells. *International Journal of Biological Macromolecules*, *275*, 133731.

Faisal, M., Iqbal, T., Usama, M., Ahmad, K., Khan, M. S., Waris, I., Raza, H., Ghafoor, R., Tahir, U. Bin, & Iftikhar, R. (n.d.). *Elucidating the Anthelmintic Efficacy and Phytochemical Profile of Citrullus colocynthis (Linnaeus) Schrader*.

Fatima, M., Iqbal, T., Shaheen, L., Salma, U., Siddique, R., Ali, R., Rehman, A. U., & Usman, S. (2023). Transmission dynamics of rabies virus. *Zoonosis, Unique Scientific Publishers, Faisalabad, Pakistan*, *3*, 386–397.

Grover, T., Mishra, R., Gulati, P., & Mohanty, A. (2021). An insight into biological activities of native cyclotides for potential applications in agriculture and pharmaceutics. *Peptides*, *135*, 170430.

Gulnaz, R., Saqib, M., Saleem, M., Fatima, M., Iqbal, T., & Arif, Z. (2023). Outbreak of the ebola virus. *Zoonosis, Unique Scientific Publishers, Faisalabad, Pakistan*, *3*, 359–373.

Han, Y., Pan, J., Ma, Y., Zhou, D., & Xu, W. (2022). Protein-based biomaterials for combating viral infections: Current status and future prospects for development. *Biosafety and Health*, *4*(2), 87–94.

Hessel, S. S., Dwivany, F. M., Zainuddin, I. M., Wikantika, K., Celik, I., Emran, T. Bin, & Tallei, T. E. (2023). A computational simulation appraisal of banana lectin as a potential anti-SARS-CoV-2 candidate by targeting the receptor-binding domain. *Journal of Genetic Engineering and Biotechnology*, *21*(1), 148.

Humaira, H. A., Iqbal, T., Habib, I., & Aman, Z. (2023). Vaccine strategies for dengue fever. *Zoonosis, Unique Scientific Publishers, Faisalabad, Pakistan*, *3*, 561–575.

Iqbal, M. U., Altaf, S., Naeem, M. A., Aufy, M., Alfuraydi, A. A., Iqbal, T., Hussein, A. M., Maksoud, M. A. A., & Malik, A. (2024). Amelioration of Organophosphate Poisoning Using Red Blood Cell Membrane-Cloaked Oil Nano-Sponge. *Journal of Biological Regulators and Homeostatic Agents*, 5753–5767. https://doi.org/10.23812/J.BIOL.REGUL.HOMEOST.AGENTS.20243808.462

Iqbal, T., Ahmad, A., Naveed, M. T., Ali, A., & Ahmad, M. (2023). Potential Role of Zoonoses in Bioterrorism. *Zoonosis, Unique Scientific Publishers, Faisalabad, Pakistan*, *1*, 499–512.

Iqbal, T., & Altaf, S. (2024). *Nigella Sativa use for the Treatment of Cancer*. https://doi.org/10.26717/BJSTR.2024.55.008660

Iqbal, T., Altaf, S., Basit, I., Naeem, M. A., Akram, Q., Saeed, M. R., Hyder, S., & Salma, U. (2024). Hesperetin: A Potent Phytochemical Constituent for the Treatment of Rheumatoid Arthritis: Hesperetin for the Treatment of Rheumatoid Arthritis. *Pakistan BioMedical Journal*, 2–10.

Iqbal, T., Altaf, S., Fatima, M., Rasheed, R., Laraib, K., Azam, M., Karamat, M., Salma, U., & Usman, S. (2024). *A narrative review on effective use of medicinal plants for the treatment of parasitic foodborne diseases. Agrobiological Records 16: 79-92*.

Iqbal, T., Altaf, S., Salma, U., Fatima, M., Khan, M. N., Farooq, S., Abrar, M., Tasleem, M., & Afzal, A. (2024). *Cell membrane coated polymeric nanocarriers: a novel drug delivery approach for the targeted therapy of rheumatoid arthritis. Agrobiological Records 15: 91-102*.

Iqbal, T., Fatima, M., & Altaf, S. (2022). *Role of Platelet Membrane Coated Nanoparticles to Treat Rheumatoid Arthritis*.

Iqbal, T., Salma, U., Umair, M., Iqbal, H., Khalid, T., & Hyder, S. (2024). Utilizing Medicinal Plants for Disease Treatment in Aquaculture: An Approach to Improve Fish Health: Medicinal Plants in Aquaculture. *MARKHOR (The Journal of Zoology)*, 3–10.

Jamal, Q. M. S. (2022). Antiviral potential of plants against COVID-19 during outbreaks—An update. *International Journal of Molecular Sciences*, *23*(21), 13564.

Lanrewaju, A. A., Enitan-Folami, A. M., Nyaga, M. M., Sabiu, S., & Swalaha, F. M. (2024). Cheminformatics bioprospection of selected medicinal plants metabolites against trypsin cleaved VP4 (spike protein) of rotavirus A. *Journal of Biomolecular Structure and Dynamics*, *42*(20), 10652–10671.

Lee, M. F., Tan, S. L., Ahemad, N., Hamid, A. A. A., Hishamuddin, S. A. S. N., Batumalaie, K., Afzal, S., & Wu, Y. S. (2024). Molecular docking and dynamics simulation reveal withanolides as potent antivirals against dengue virus. *South African Journal of Botany*, *169*, 426–434.

Lian, X., Yang, X., Yang, S., & Zhang, Z. (2021). Current status and future perspectives of computational studies on human–virus protein–protein interactions. *Briefings in Bioinformatics*, *22*(5), bbab029.

Liang, D., Xiao, C., Song, F., Li, H., Liu, R., & Gao, J. (2021). Complete Genome Sequence and Function Gene Identify of Prometryne-Degrading Strain Pseudomonas sp. DY-1. *Microorganisms*, *9*(6), 1261.

Mammari, N., Krier, Y., Albert, Q., Devocelle, M., Varbanov, M., & OEMONOM. (2021). Plant-derived antimicrobial peptides as potential antiviral agents in systemic viral infections. *Pharmaceuticals*, *14*(8), 774.

Muhseen, Z. T., Ahmad, S., & Li, G. (2021). Structural basis of UDP-N-acetylglucosamine pyrophosphorylase and identification of promising terpenes to control Aedes aegypti. *Colloids and Surfaces B: Biointerfaces*, *204*, 111820.

Mushtaq, H., Zahid, H., Ahmad, D., Sattar, A., & Iqbal, T. (n.d.). *Efficacy of Homeopathic Therapy in Arthritis Treatment*.

Nandu, T. G., & Jithesh, K. (2024). Natural Product-Based Anti-Viral Agents Against RNA Viruses: An Important Strategy for Pandemic Preparedness. In *Drugs from Nature: Targets, Assay Systems and Leads* (pp. 411–440). Springer.

Ojha, R., Kaur, S., Sinha, K., Chawla, K., Kaur, S., Jadhav, H., Kaur, M., & Bhunia, R. K. (2021). Characterization of oleosin genes from forage sorghum in Arabidopsis and yeast reveals their role in storage lipid stability. *Planta*, *254*, 1–12.

Patel, B., Sharma, S., Nair, N., Majeed, J., Goyal, R. K., & Dhobi, M. (2021). Therapeutic opportunities of edible antiviral plants for COVID-19. *Molecular and Cellular Biochemistry*, *476*, 2345–2364.

Ramesan, C. K. V, Vinod, N. V, & Skariyachan, S. (2023). 1Department of Microbiology, Sree Narayana College, Kannur, Kerala, India, 2Department of Microbiology, St. Pius X College, Kasaragod, Kerala, India. *Antimicrobial Peptides*, 261.

Saleem, F., Atiq, A., Altaf, S., Habib, M., & Iqbal, T. (2023). Etiology, treatment and complications of dengue fever: a systematic analysis. *Zoonosis, Unique Scientific Publishers, Faisalabad, Pakistan*, *3*, 551–560.

Saleem, M., Munir, R., Aslam, T., Altaf, S., & Aziz, A. (n.d.). *Mathematical Pharmacokinetics and Drug Delivery*.

Salma, U., Nawaz, H., Farooq, M., & Iqbal, T. (2023). Management, control and treatment of monkeypox disease. *Zoonosis, Unique Scientific Publishers, Faisalabad, Pakistan*, *3*, 666–675.

Saqib, M., Iqbal, K. J., Khan, S., Gulnaz, R., Iqbal, T., Mankga, L. T., & Fatima, K. (2023). Immune boosters to combat zoonotic viral diseases. *Zoonosis, Unique Scientific Publishers, Faisalabad, Pakistan*, *3*, 344–358.

Shaker, B., Ahmad, S., Lee, J., Jung, C., & Na, D. (2021). In silico methods and tools for drug discovery. *Computers in Biology and Medicine*, *137*, 104851.

Siew, Z. Y., Asudas, E., Khoo, C. T., Cho, G. H., Voon, K., & Fang, C.-M. (2024). Fighting nature with nature: Antiviral compounds that target retroviruses. *Archives of Microbiology*, *206*(3), 130.

Szerszunowicz, I., & Kozicki, S. (2023). Plant-derived proteins and peptides as potential immunomodulators. *Molecules*, *29*(1), 209.

Tasleem, F., Shahzadi, S., Bassey, O. B., Shuja, A. A., Ali, M., Bibi, S., Ahmed, T., Hameed, M. K., & Altaf, S. (2025). 6-Amino flavone attenuates cadmium-induced memory impairment and neuroinflammation through p-JNK/NF-κB pathway inhibition in mice. *Journal of Medical & Health Sciences Review*, 2(2), 3615–3633**.**

Thomas, E., Stewart, L. E., Darley, B. A., Pham, A. M., Esteban, I., & Panda, S. S. (2021). Plant-based natural products and extracts: Potential source to develop new antiviral drug candidates. *Molecules*, *26*(20), 6197.

Umair, M., Altaf, S., Muzaffar, H., Iftikhar, A., Ali, A., Batool, N., Iqbal, T., & Saif-ur-Rehman, B. S. R. (2022). Green nanotechnology mediated silver and iron oxide nanoparticles: Potential antimicrobials. *Agrobiol Rec*, *10*, 35–41.

Wang, J., Wu, Y., Deng, X., & Zhang, L. (2024). A GRFT-like method for highly maneuvering target detection via neural network. *IEEE Geoscience and Remote Sensing Letters*.