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Molecular Docking Analysis Reveals the Antiviral Potential of Oleanane Against Potato Virus Y Infection Affecting the Growth of *Solanum tuberosum*

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Abstract

Potatoes (*Solanum tuberosum*) are the world's third-most significant food crop for human consumption, with notable contributions to global food security and nutrition. In India, potatoes are extensively cultivated, yielding high carbohydrate, fibre, and vitamin content per unit area compared to other staple crops like rice and wheat. Despite significant production, potato yields are severely impacted by various biotic stressors, including viral infections. Over 40 viruses affect potatoes globally, with Potato Leaf Roll Virus (PLRV), Potato Virus Y (PVY), and Potato Virus X (PVX) being the most detrimental. The objective of these studies is to find out the antiviral plant-based compound that has therapeutic potential against Potato virus Y. The causative genes in potato virus Y were retrieved through Cytoscape cross-species network analysis. Further, the network was analysed for the identification of the priority gene using 12 different parameters on CytoHubba. The 'Nlb' gene was identified as the priority gene affected in potato virus Y. "Nlb" is a PVY-affected gene that is essential to the virus's propagation and replication inside the plant, which influences the plant's susceptibility to the infection. Further, to identify the bio pesticide that can be effective against potato virus Y, a list of antiviral phytochemicals was curated through intense literature study. These phytochemicals were screened on the basis of Lipinski's rule of 5 using ADMETLab 3.0. The molecular docking studies between the phytochemicals and the identified priority gene revealed the therapeutic potential of "Oleanane" against potato virus Y. Therefore, Oleanane is the best plant-based therapeutics compound and obtained from soya bean (*Glycine max*), Sal tree, as eco-friendly compounds for viral diseases in potatoes.

Keywords: Network Pharmacology, Nlb, Oleanane, Potato Leafroll Virus (PLRV), Potato Virus Y (PVY)

1. Introduction

Potatoes (*S. tuberosum*), after rice and wheat, are currently the world's third-most significant food crop for human consumption; more than half of its production is currently done in developing nations[1]. With an average productivity of roughly 17.19 tonnes/ha, 19.13 million hectares of land are used to produce approximately 328.87 million tons of potatoes worldwide. With a production of approximately 25 million tonnes and a productivity of 17.86 tonnes/ha, potatoes are grown on roughly 1.4 million hectares of land in India[2]. Thousands of years passed until the Incas established their empire in the area that is now Peru, Chile, and Bolivia in 1532. A single kind of potato that is produced in Southern Peru is the source of all cultivated potatoes. India, behind China and Russia, is the world's

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third-largest producer of potatoes. Potatoes were brought from Europe to India early 17th century. It has been farmed commercially due to the fact 18302. Compared to rice and wheat, which yield 2. Five and 1.0 kg of fit-to-be-eaten protein/ha/day, potatoes yield three kg. In contrast to different important food vegetation, potatoes yield better amounts of carbohydrates, fibre, and vitamins per unit[3].

Potatoes yield more nutrient-dense food per unit of land and time than many other crops. Potatoes contain 80% water by weight when they are fresh, and they provide 90-100 calories per 100g[4]. Potatoes are a good source of small molecules and secondary metabolites, in addition to being high in starch. These molecules are crucial in many different processes[5]. Many of the substances found in potatoes are significant due to their positive health effects, making them extremely desirable for inclusion in a person's diet[6]. In the nations where potatoes constitute the staple meal, nutritional deficiencies are not well recognized[7]. Increasing the amount of nutrients available to a big portion of the worldwide population is one of the goals of global health. Increasing the nutritional value of popular crops would be a smart way to accomplish this goal. Potatoes are cultivated and consumed in vast quantities all over the world. Moreover, potatoes can be developed through breeding and biotechnology methods and have better phytonutrient content[8].

Over 80% of the potato crop in north India's vast Indo-Gangetic plains is grown during the brief winter season of October through March. Approximately 8% of the land used for potato production is in the hills, where the crop is grown over the long summer months of April through October. Potatoes are farmed as an irrigated Rabi crop in the winter (November to March) or as a rainfed Kharif crop during the rainy season (July to October) in the plateau regions of South-Eastern, Central, and Peninsular India, which make up around 6% of the total area. Approximately 73% of India's cropland and 80% of the country's overall output are found in the states of Uttar Pradesh, West Bengal, and Bihar[9]. Potato production in Uttar Pradesh was 11.09 million tons in 2007-2008, with 0.42 million ha under cultivation[10].

Potato output is poor per unit area due to many biotic and abiotic stressors, including viruses, even with the introduction of high yielding varieties and enhanced cultural methods. The crop's potential yield is significantly reduced by viral infections. Upon encountering viral pathogens, plants initially undergo molecular reactions that trigger a variety of physiological responses, including changes in respiration, photosynthesis rate, hormone concentrations, and the build-up of proteins and signal molecules linked to pathogenesis. More than 40 viruses naturally infect potatoes worldwide[11]. Potato Leafroll Virus (PLRV, genus *Polierovirus*), Potato Virus X (PVX, genus *Potexvirus*), Potato Virus A and Y (PVA, PVY, both genus *Potyviruses*), and Potato Virus S (PVS, genus *Carlavirus*) are some of the most frequent viruses that impact potato crops[12]. The sources and vectors of virus transmission are fungus, seeds, and insects (aphid, beetle, leaf hopper, and whitefly)[13]. While mild strains of potato viruses X, S, A, and M may lower yields by 10-30%, severe strains of potato virus Y and leaf roll may cause a 60-75% loss in tuber yield[14,15]. Extended utilization of out-dated, contaminated seed stocks for three to four years reduced their yielding capacity to over fifty per cent[14,15,16]. The disease has become uncontrollably widespread due to PVY; the primary cause of the large yield losses in potato production is the isolates of PVY that cause severe symptoms on potato tubers of susceptible cultivars[17].

Potato virus Y disease on potato plants, known also as one of the causes of potato degeneration, was recorded at the beginning of the twentieth century[17]. Several errors can be identified in the sequence when the PVY RNA genome is replicated, which could result in the emergence of novel isolates[18]. Furthermore, recombination processes caused by RNA viruses frequently result in the interchange of genetic material across isolates, adding to the heterogeneity of the viral sequence[19,20,21]. Potato Virus Y (PVY) is a type of member of the biggest plant viral group, the genus *Potyvirus*, which mostly affects species in the *Solanaceae* family. The PVY genome consists of a single-stranded (+) RNA approximately 9,700 nucleotides in length, expressed as a single polyprotein. This polyprotein undergoes auto-enzymatic cleavage to produce 10 functional proteins: VPg (genome-linked protein), NIa (small nuclear inclusion protein), NIb (large nuclear inclusion protein), P1 (first protein), HC or HC-Pro (helper component protein), P3 (third protein), 6K1 (first 6 kDa protein), CI (cytoplasmic inclusion protein), 6K2 (second 6 kDa protein), and CP (coat protein). There are two distal noncoding regions, 50 NTr and 30 NTr, on either end of the PVY genome[22]. With respect to its scientific and commercial significance, PVY, one of the most significant potato viruses, is ranked as the fifth most significant plant virus globally[23]. It can spread naturally through contaminated "seed" materials, aphid vectors, mechanical contact, or artificial laboratory propagation. Additionally, reports of seed transmission exist[17]. PVY is spread by a variety of aphid vectors

belonging to the *Aphidinae* family in a nonpersistent way. *Myzuspersicae* is the species that spreads PVY the most efficiently, but *Macrosiphum euphorbiae* is also important[24].

2. Materials and Methods

2.1 Protein-Protein Interaction Analysis

STRING: cross-speciesquery was used to generate a STRING network between Potato Virus Y and *S. tuberosum* to study protein-protein interaction networks. Further, cytoHubba plugin of Cytoscape was used to analyse the hub genes in the network at different parameters like MCC, DMNC, MNC, DEGREE, EPC, Bottleneck, EcCentricity, Closeness, Radiality, Betweenness, Stress, and Clustering Coefficient. The resulting protein-protein interaction network were analysed to identify the common priority gene among the different interaction networks.

2.2 3D Structural Modeling

The 3D structure of the priority gene identified through the protein-protein interaction network was modelled using the SWISS-MODEL tool.

2.3 Library Preparation and Virtual Screening

An intensive literature study was done to identify the phytochemical with antiviral potential. The PubChem database was used to obtain the canonical SMILES, names, and sources of these compounds. A library of 29 antiviral phytochemicals was prepared. In order to generate a library of possible lead compounds, phytochemicals were screened virtually on the basis of Lipinski's rule of five using ADMETLab 3.0.

2.4 Molecular Docking

SeamDock was used to carry out molecular docking studies of the target protein and the phytochemicals. The target protein structure modelled using SWISS-MODEL was used for the molecular docking studies. Molecular docking studies estimate the binding affinity of the phytochemicals with the target protein. The docking parameters were set to; spacing = 0.375, mode number = 10, energy range = 5, Exhaustiveness = 8.

3. Result

3.1 Identification of Target Protein using Protein-Protein Interaction Studies

The network analysis, using 12 different parameters (MCC, DMNC, MNC, DEGREE, EPC, Bottleneck, EcCentricity, Closeness, Radiality, Betweenness, stress, Clustering Coefficient) (Figure 2) identified the "Nlb" gene as the priority gene (Table 1) as the key gene at 0.4 confidence level.

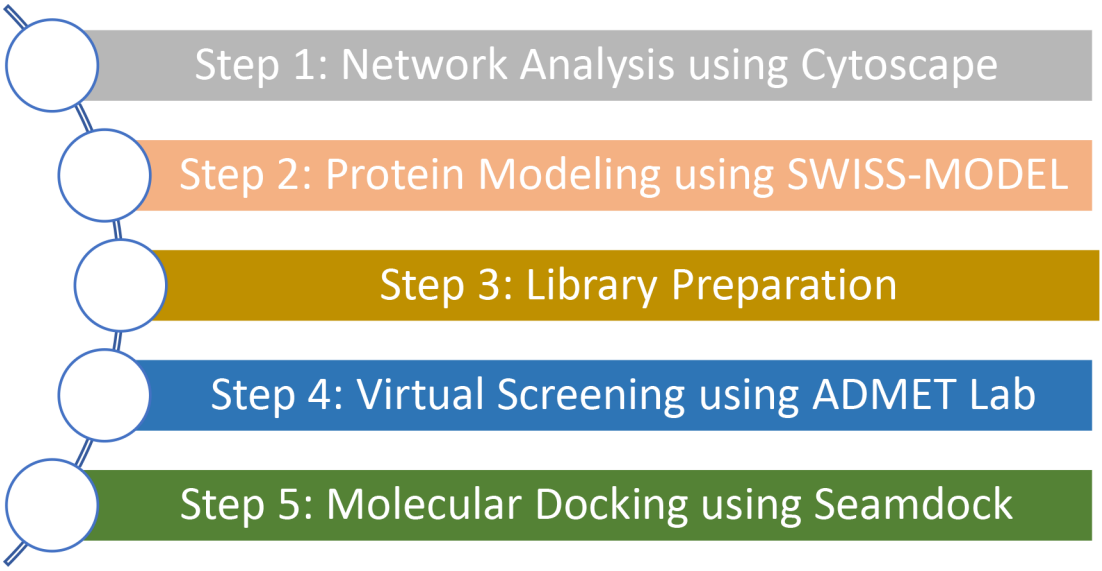


Figure 1. Flowchart representing the steps of the methodology of the study.

3.2 Protein Modeling

The 3D structure of Nlb protein was modelled through SWISS-MODEL (Figure 3). The sequence of the protein was retrieved from Cytoscape.

"Nlb" protein sequence retrieve from the Cytoscape.

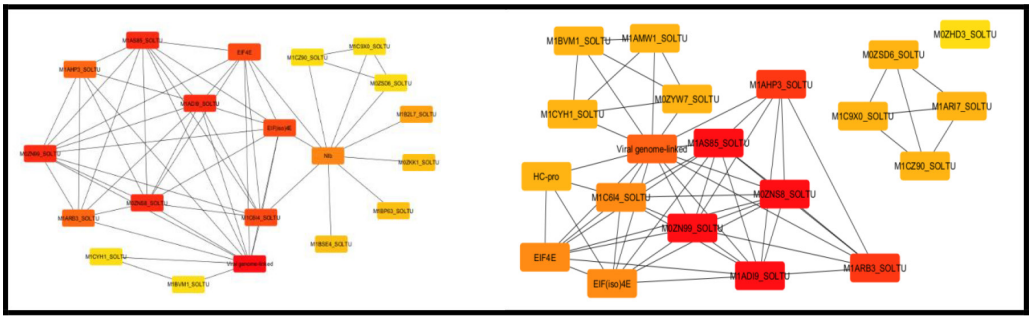
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YSKPIDVGVVDRMHLRKPSIGLSSTCNVHGFKKCAYVTDEQEIFKALNMKAAVGASYGCKKKDYFEHFTDADKEEIV
MQSCLRLYKGLLGIWNGSLKAELRCKEKILANKTRTFTAAPLDTLLGGKVCVDDFNNQFYSKNIECCWTVGMTKFYG
GWDKLLRRLPENWVYCDADGSQFDSSLTPYLINAVLTIRSTYMEDWDVGLQMLRNLYTEIVYTPISTPDGTIVKKFRG
NNSGQPSTVVDNSLMVVLAMHYALIKECVEFEEIDSTCVFFVNGDDLLIAVNPEKESILDRMSQHFSDLGLNYDFSSRT
RRKEELWFMSHRGLLIEGMYVPKLEEERIVSILQWDRADLPEHRLEAICAAMIESWGYSELTHQIRRFYSWLLQQQPFA
TIAQEGKAPYIASMALRKLYMDRAVDEEELRAFTEMMVALDDEFELDSYEVHHQ

3.3 Library Preparation and Virtual Screening

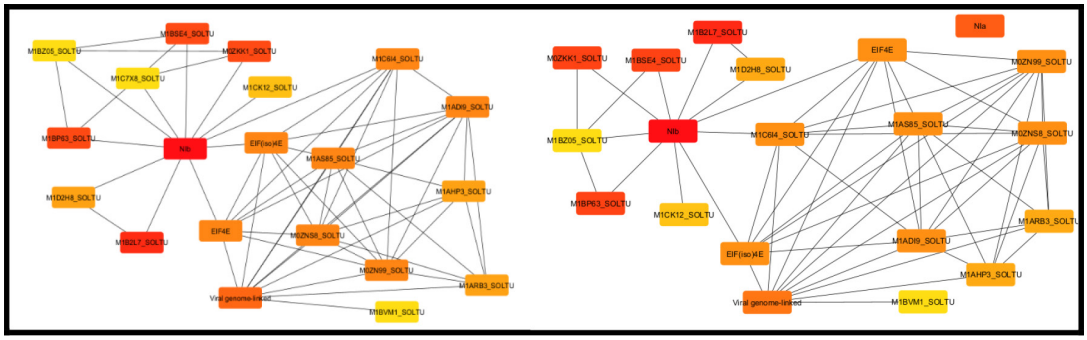
A total of 29 antiviral phytochemicals were listed through literature review and PubChem. The phytochemicals were screened based on Lipinski's

Table 1. Hub genes identified at different parameters through CytoHubba plugin of Cytoscape

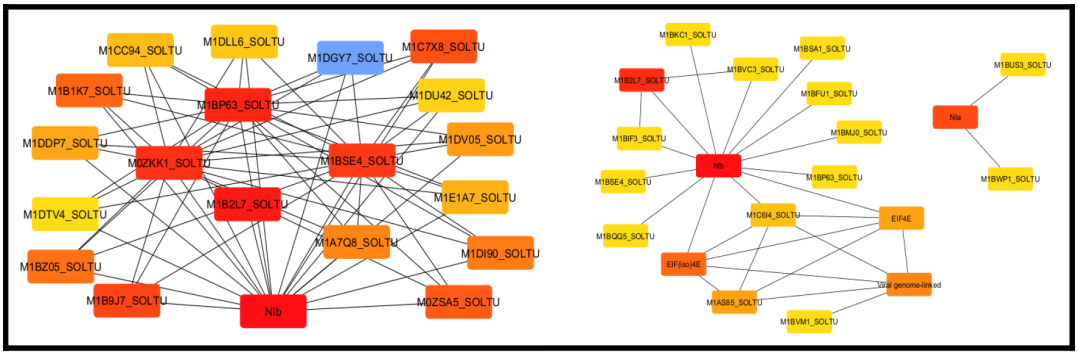
MCC	DMNC	MNC	Degree	EPC	Bottl eneck	EcCentr	Closen ess	Radialit y	Betwee nness	Stress
NIb	HC-pro	Nib	NIb	NIb	NIb	NIb	NIb	NIb	NIb	NIb
Viral genom elinked	Viral genome linked	Viral genome linked	Viral genome linked	M1AHQ0_ SOLTU	Viral genome linked	Viral genome linked	M1BP63_ SOLTU	M1BP63_ SOLTU	Viral genome linked	NIa
M1ARB3_ SOLTU	M1ARB3_ SOLTU	M1ARB3_ SOLTU	NIa	M1BP63_ SOLTU	NIa	HC-pro	M1C9X0_ SOLTU	M1C9X0_ SOLTU	NIa	Viral genomelinked
M1BP63_ SOLTU	M1C9X0_ SOLTU	M1BP63_ SOLTU	M1ARB3_ SOLTU	M0ZKK1_ SOLTU	M1B2L7_ SOLTU	M1BP63_ SOLTU	M0ZKK1_ SOLTU	M0ZKK1_ SOLTU	M1BP63_ SOLTU	M1BP63_ SOLTU
M1C9X0_ SOLTU	M1ARI7_ SOLTU	M0ZKK1_ SOLTU	M1BP63_ SOLTU	M1DU42_ SOLTU	M1BKC1_ SOLTU	M1BQQ5_ SOLTU	M1B2L7_ SOLTU	M1B2L7_ SOLTU	M0ZKK1_ SOLTU	M0ZKK1_ SOLTU
M0ZKK1_ SOLTU	M1CZ90_ SOLTU	M1B2L7_ SOLTU	M0ZKK1_ SOLTU	M1B2L7_ SOLTU	M1BIF3_ SOLTU	M1BSA1_ SOLTU	StCDPK6	StCDPK6	M1B2L7_ SOLTU	M1B2L7_ SOLTU
M1B2L7_ SOLTU	M1ADI9_ SOLTU	M1ADI9_ SOLTU	M1B2L7_ SOLTU	M1DV05_ SOLTU	M1BSE4_ SOLTU	M1ADI9_ SOLTU	M1CZ90_ SOLTU	M1CZ90_ SOLTU	StCDPK6	M1ADI9_ SOLTU
M1CZ90_ SOLTU	M0ZYW7_ SOLTU	M1AS85_ SOLTU	M1ADI9_ SOLTU	M1BSE4_ SOLTU	M1BQQ5_ SOLTU	M1AS85_ SOLTU	M1DC90_ SOLTU	M1DC05_ SOLTU	M1ADI9_ SOLTU	M1AS85_ SOLTU
M1ADI9_ SOLTU	M1AS85_ SOLTU	M1BSE4_ SOLTU	M1AS85_ SOLTU	M1A7Q8_ SOLTU	M1AS85_ SOLTU	M1BSE4_ SOLTU	M1BSE4_ SOLTU	M1BSE4_ SOLTU	M1AS85_ SOLTU	M1BSE4_ SOLTU
M1AS85_ SOLTU	M0ZN99_ SOLTU	M0ZN99_ SOLTU	M1BSE4_ SOLTU	M1DGY7_ SOLTU	M1BP63_ SOLTU	M0ZN99_ SOLTU	M1Bz05_ SOLTU	M1BZ05_ SOLTU	M1BSE4_ SOLTU	M0ZN99_ SOLTU
M0ZN99_ SOLTU	M1AMW1_ SOLTU	M1BZ05_ SOLTU	M0ZN99_ SOLTU	M1CB05_ SOLTU	EIF4E	M1BVC3_ SOLTU	EIF4E	M1CB05_ SOLTU	M0ZN99_ SOLTU	M1BZ05_ SOLTU



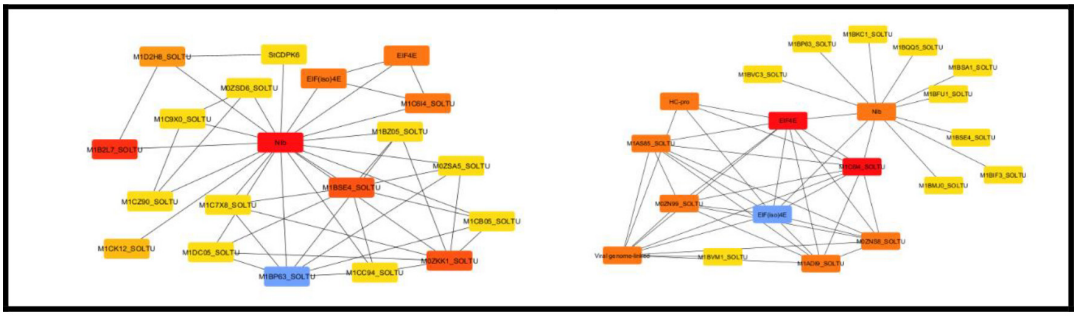
(A) **(B)**


M1BSE4_SOLTU
M1BZ05_SOLTU
M0ZKK1_SOLTU
M1C7X8_SOLTU
M1CK12_SOLTU
M1C6I4_SOLTU
M1AD9_SOLTU
M1BP63_SOLTU
Nlb
EIF(iso)4E
M1AS85_SOLTU
M1AHP3_SOLTU
M1D2H8_SOLTU
EIF4E
M0ZNS8_SOLTU
M1BZL7_SOLTU
M0ZN99_SOLTU
M1ARB3_SOLTU
Viral genome-linked
M1BVM1_SOLTU
Nla
M1ADI9_SOLTU

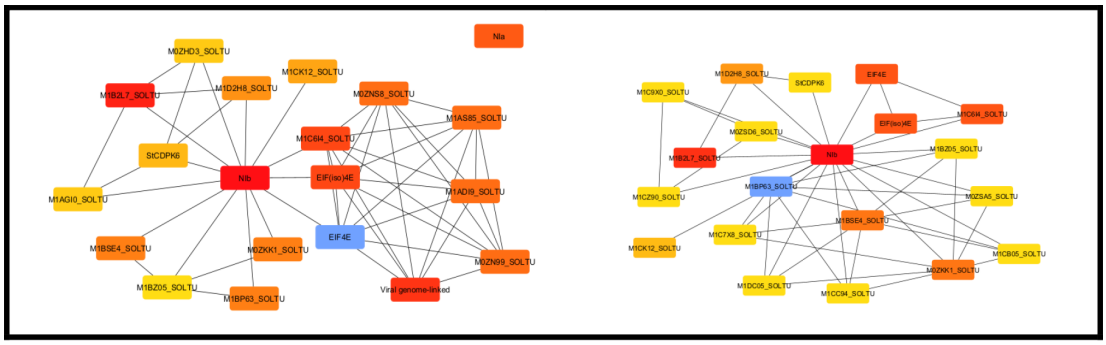
(C) (D)


M1CC94_SOLTU
M1DLL6_SOLTU
M1DGY7_SOLTU
M1C7X8_SOLTU
M1B1K7_SOLTU
M1BP63_SOLTU
M1DU42_SOLTU
M1DDP7_SOLTU
M1DV05_SOLTU
M0ZKK1_SOLTU
M1BSE4_SOLTU
M1B2L7_SOLTU
M1E1A7_SOLTU
M1DTV4_SOLTU
M1A7Q8_SOLTU
M1DI90_SOLTU
M1BZ05_SOLTU
M1B9J7_SOLTU
Nlb
M0ZSA5_SOLTU
M1BKC1_SOLTU
M1BSA1_SOLTU
M1BVC3_SOLTU
M1BUS3_SOLTU
M1BFU1_SOLTU
Nla
M1BIF3_SOLTU
M1BMJ0_SOLTU
M1BWP1_SOLTU
M1BQQ5_SOLTU
M1BVM1_SOLTU

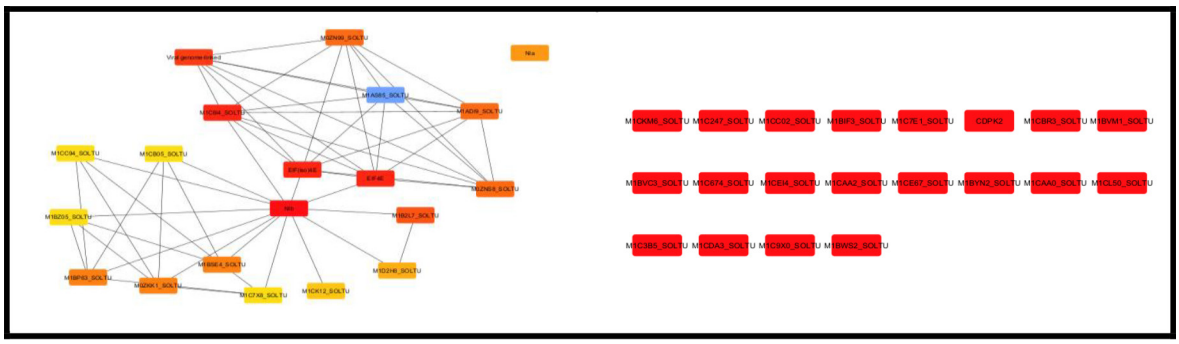
(E) (F)


M1D2H8_SOLTU
StCDPK6
EIF4E
EIF(iso)4E
M0ZSD6_SOLTU
M1C6I4_SOLTU
M1C9X0_SOLTU
Nlb
M1BZ05_SOLTU
M1BZL7_SOLTU
M0ZSA5_SOLTU
M1CZ90_SOLTU
M1C7X8_SOLTU
M1BSE4_SOLTU
M1CB05_SOLTU
M1CK12_SOLTU
M1DC05_SOLTU
M0ZKK1_SOLTU
M1BP63_SOLTU
M1CC94_SOLTU
HC-pro
M1BVM1_SOLTU
M1ADI9_SOLTU
M0ZN99_SOLTU
M1BMJ0_SOLTU
M1BIF3_SOLTU

(G) (H)


M0ZHD3_SOLTU
M1CK12_SOLTU
M1BZL7_SOLTU
M1D2H8_SOLTU
M0ZNS8_SOLTU
M1AS85_SOLTU
M1C6I4_SOLTU
StCDPK6
Nlb
EIF(iso)4E
M1ADI9_SOLTU
M1AGI0_SOLTU
EIF4E
M1BSE4_SOLTU
M0ZKK1_SOLTU
M0ZN99_SOLTU
M1BZ05_SOLTU
M1BP63_SOLTU
Viral genome-linked
Nla
M1D2H8_SOLTU
StCDPK6
EIF4E
M1C9X0_SOLTU
M1C6I4_SOLTU
EIF(iso)4E
M0ZSD6_SOLTU
M1BZL7_SOLTU
Nlb
M1BZ05_SOLTU
M1CZ90_SOLTU
M1BP63_SOLTU
M0ZSA5_SOLTU
M1BSE4_SOLTU
M1C7X8_SOLTU
M1CK12_SOLTU
M1CB05_SOLTU
M0ZKK1_SOLTU
M1DC05_SOLTU
M1CC94_SOLTU

(I) (J)



(K) **(L)**

Figure 2 Protein-protein interaction network constructed on cytoscape using different parameters, **(A)** MCC **(B)** DMNC **(C)** MNC **(D)** Degree **(E)** EPC **(F)** Bottleneck **(G)** EcCentricity **(H)** Closeness **(I)** Radiality **(J)** Betweenness **(K)** Stress **(L)** Clustering Coefficient.

Table 2. List of phytochemicals retrieved from the study along with their plant source and Lipinski's rule of 5 statuses

Phytochemicals	Class	Plant (Part)	Lipinski Rule
Chalcones	Ketone	*Glycyrrhiza inflate* (roots)	Accepted
Dammarenolic acid	Triterpenoid	*Aglaia sp.* (bark)	Accepted
Decanoylphorbol-13 acetate	Diterpene	*Croton mauritianus* (leaves)	Accepted
Loliolide	Tannins	*Phyllanthus urinaria* (whole plant)	Accepted
Honokiol	Lignin	*Magnolia tree* (roots, bark)	Accepted
Oleanane	Triterpenes	*Camellia japonica* (flowers)	Accepted
Quercetin	Flavonoid	*Embelia ribes*(seeds)	Accepted
SJP-L-5	Lignin gomisin	*Schisandra micrantha* (roots)	Accepted
Xanthohumol	Chalcone	*Humulus lupulus*(wholeplant)	Accepted
Oxyresveratrol		*Artocarpus lakoocha* (Heartwood)	Accepted
Pterocarpan A		*Pterocarya stenoptera* (Bark)	Accepted
LPRP-Et-97543		*Liriope platyphylla*(Root)	Accepted
5,7,4' trihydroxy-8methoxyflavone (F36)		*Scutellaria baicalensis*(Root)	Accepted
Isobavachalcone	chalcones	*Morus cathayana, Hypericum geminiflorum,*	Accepted
Betulinic Acid		*Paeoniaemodi, Bowdichia virgilioides,*	Accepted
Rosmarinic Acid		*Salvia miltiorrhiza, Aspergillus duricaulis,*	Accepted
Berberine			Accepted
Lapachol		*Catalpa ovata, Plenckia populnea*	Accepted
Thymol		*Acanthospermum australe, Humulus lupulus,*	Accepted
Allicin		*Allium ursinum, Allium ampeloprasum*	Accepted
Saikosaponins	Terpenoid	*Bupleurum kaoi* (roots)	Rejected
Sennoside A	Glycoside	*Rheum palmatum* (roots)	Rejected
Silvestrol	Benzofuran	*Aglaia foveolata* (leaves, bark)	Rejected
Excoecarianin	Tannins	*Phyllanthus urinaria* (whole plant)	Rejected
Glycyrrhizic acid		*Glycyrrhizae radix* (Roots)	Rejected
Dicaffeoylquinic acids		*Schefflera heptaphylla* (Leaf stalks)	Rejected
Hypericin		*Hypericum ascyron, Hypericum tomentosum*	Rejected
Oleuropein			Rejected
Baicalin	Flavonoid	*Scutellaria baicalensis* (roots)	Rejected

rule of five using ADMETLab 3.0. Out of 29 antiviral phytocompounds 20 follow Lipinski's rule of five. Here Table 2 represents phytochemicals with Lipinski's rule accepted or rejected.

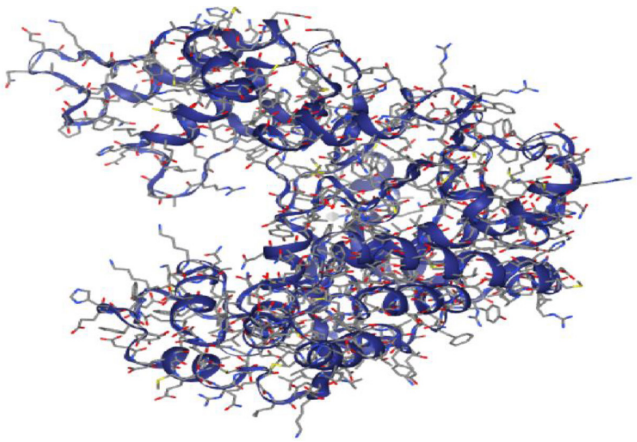


Figure 3. 3D protein structure of Nlb gene generated by SWISS-MODEL.

3.4 Molecular Docking

The molecular docking of Nlb protein was done with the 20 screened phytochemicals. Oleanane showed strong therapeutic promise against PVY based on molecular docking experiments between the screened phytochemicals and the "Nlb" protein (Figure 4). Oleanane's strong binding affinity (-9.1 kcal/mol) for the "Nlb" protein in docking studies suggests it is potential efficacy against potato virus Y (Table 3).

4. Discussion

In this study, we identified important genes and possible treatment drugs against Potato Virus Y (PVY) by combining a variety of molecular modelling techniques and bioinformatics tools. Our method combined virtual screening, molecular docking investigations, network analysis, 3D protein structure modelling, and a comprehensive study of the literature on antiviral phytochemicals. We have determined that

Table 3. List of phytochemicals and their amino acid residues and binding energy with the Nlb protein

Compound	Binding Energy	Amino Acid Residues
Chalcones	-6.58	I436,M440,I441,L461,T468,P476,Y477,L483,L483,L486
Dammarenolic acid	-7.94	L177,R178,I183,W423,R425,E176
Decanoylphorbol-13 acetate	-5.35	R455,W459,Q462,I469,K474,A475,S458,E472
Loliolide	-5.94	Y78,T190,T192,P295,K306,Y71,N310,S312
Honokiol	-6.48	P429,E430,L460,Q464,Q463,Q422,D424,R432
Oleanane	-9.1	N125,A128,F191,A194,L199,P315
Quercetin	-6.54	K77,T190,K73,D74,T188,D255,D255,Q253,R189
SJP-L-5	-6.17	D88,T259,Y261,V87
Xanthohumol	-5.44	D74,T190,D255,Y78,T188,Q253,K182,R189
Oxyresveratrol	-7	L124,N125,F191,A194,L199,P315,K138,G313,A193
Pterocarpan A	-7.06	F191,L199,T317,K138,V318,A194,G313,P315
LPRP-Et-97543	-6.72	E430,I436,L460,L461,Q463,Q464,D424,R432,P429,P 465
5,7,4' trihydroxy-8methoxyflavone (F36)	-6.48	D424,P429,L460,Q463,Q464,Q422,R432,W423
Isobavachalcone	-6.58	P241,W244,V245,R389,R390,K391,L403,Y408,Y246 ,E392,
Betulinic Acid	-8.36	R178,L177,I183,W423,C179
Rosmarinic Acid	-6.15	K138,A128,A129,F191,A193,L199,S312,Q314,A194,
Allicin	-4.33	T102,V348,F350,C347,F349
Berberine	-7.16	D74,Y78,R189,T190,Q253,S312,D255,
Lapachol	-5.97	A128,A129,F191,A193,L199,K138,A194,G313,
Thymol	-5.78	K80,I82,R308,D83,S257,

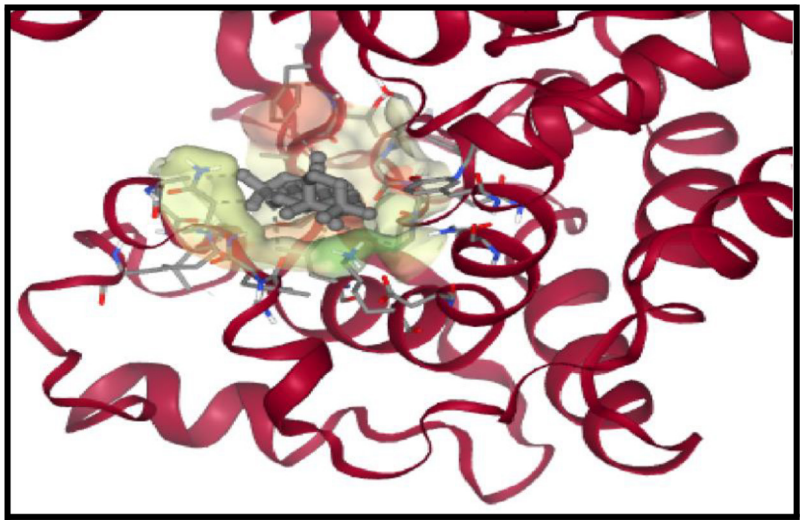


Figure 4. Molecular docking interaction of Oleanane phytochemicals with Nlb protein (hub gene).

the phytochemical "Oleanane" and the gene "Nlb" are important targets because of our thorough investigation. Recent studies that have identified novel therapeutic targets in plant virology have demonstrated the importance of such a multidisciplinary approach[25,26].

Numerous plants contain pentacyclic triterpene oleanane, which is well-known for its diverse biological effects[27]. Oleanane is a promising candidate for medicinal uses because of studies that demonstrate its antiviral, anti-inflammatory, and anticancer qualities[28,29,30]. Its special structure, which enables it to interact with biological targets in ways that can impede virus multiplication and dissemination, is primarily responsible for these advantageous effects.

When it comes to PVY infection, the "Nlb" gene is essential, especially for the way the virus replicates and spreads inside the host plant. According to research, if this gene is targeted, the virus's life cycle may be disrupted, potentially reducing the plant's susceptibility to infection[31]. Our research focuses on the Nlb gene to interfere with the essential molecular pathways that allow PVY to infect and damage potato crops.

This study integrates computational and experimental methodologies to create the foundation for creating efficient antiviral therapies to protect potato crops from PVY. Targeting the Nlb gene and identifying oleanane as a possible treatment drug present a viable strategy for lessening PVY's negative effects on agriculture. In locations where potato growing is a major sector, these tactics are essential for increasing crop yields and guaranteeing food security. This strategy is in line with recent developments in plant virology research, which highlight the need to improve crop protection by combining computational tools with conventional experimental techniques[31,32].

5. Conclusion

The research objective was to find plant-based antiviral compounds that could be used to treat Potato Virus Y (PVY). Many important steps were accomplished by combining molecular modeling and bioinformatics in an integrated manner. Using STRING and CytoHubba, a cross-species network study between PVY and *Solanum tuberosum* was carried out, and the results showed that the "Nlb" gene had an impact on the potatoes. The protein sequence for the "Nlb" gene was then retrieved using Cytoscape, and the SWISS-MODEL tool was utilized to create three-dimensional protein structures that were necessary for additional docking investigations. A thorough literature study and data extraction from PubChem resulted in the compilation of 29 antiviral phytochemicals into a library. Following Lipinski's rule of five screening of these phytochemicals with ADMETLab 3.0, 20 compounds with advantageous pharmacokinetic and pharmacodynamic properties were identified. Molecular docking examinations using SeamDock revealed that "Oleanane" had the lowest binding energy (-9.1 kcal/mol) and the best binding affinity with the "Nlb" protein, these points toward a potent antiviral effect against PVY. These findings highlight the potential of Oleanane as a biopesticide against

PVY and show the synergistic effects of molecular modeling, virtual screening, and bioinformatics in the development of plant-based antiviral drugs. The results pave the way for further experimental validation and potential development of oleanane as a sustainable strategy to enhance the health and productivity of potato crops.

6. References

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