

# Hantavirus Reservoirs in Human-to-Human Transmission: Deep Learning Frameworks for the Identification of Molecular Inhibitors Targeting and Virus Interhuman Pathogenesis

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## Abstract:

Hantaviruses are serious emerging zoonotic RNA viruses, which are associated with two major diseases (hemorrhagic fever with renal syndrome, HFRS and hantavirus cardiopulmonary syndrome, HCPS) and are maintained mainly in rodent hosts. Of the hantaviruses, Andes virus (ANDV) has been shown to be capable of human-to-human transmission, and is thus of particular public health interest. In the present study, the role of hantavirus reservoirs in Andes virus transmission is explored and Deep Learning computational techniques are used to find molecular inhibitors that inhibit viral pathogenesis. An in-silico research design was used which involves epidemiological analysis, bioinformatics, molecular docking, virtual screening, molecular dynamics simulation, and artificial intelligence supported drug discovery. The glycoproteins (Gn/Gc), nucleocapsid proteins, fusion proteins, and the RNA-dependent RNA polymerase are targeted as therapeutic proteins. The antiviral prediction and compound screening are based on deep learning frameworks like CNN, RNN, GNN and transformer-based models. Results show that transformer-based models and graph neural network models give the maximum prediction accuracy. Several compounds are identified by molecular docking studies that have high binding affinity towards Andes virus proteins. The researchers conclude that AI-enabled computational approaches could greatly enhance the discovery and development of antiviral drugs to treat novel hantavirus infections.

**Keywords:** Hantavirus, Andes virus, Human-to-human transmission, Deep learning, Molecular inhibitors, Computational virology, Molecular docking, Antiviral drug discovery

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## 1. INTRODUCTION

Hantaviruses are emerging zoonotic RNA viruses, and are mainly maintained in rodents. Human infection is typically via aerosolized urine, saliva or feces of infected rodents<sup>1</sup>. These viruses can cause serious illness in humans such as hemorrhagic fever with renal syndrome (HFRS) and hantavirus cardiopulmonary syndrome (HCPS) which are both associated with high morbidity and mortality<sup>2</sup>. The Andes virus (ANDV) has been the most studied of the hantaviruses due to its unique ability to transmit to humans from person to person, especially in South American countries like Argentina and Chile<sup>3</sup>.

### 1.1. Background Information

Eco-social and environmental conditions that influence the dynamics of rodent populations and persistence of the virus play a significant role in the epidemiology of hantavirus infections<sup>4</sup>. The principal reservoir host of Andes virus (ANDV) is the long-tailed pygmy rice rat (*Oligoryzomys longicaudatus*) and environmental shifts, like climate change, deforestation, urbanization, and agricultural development, can also elevate exposure of humans to infected rats and enhance the spread of the virus<sup>5</sup>. Andes virus has been shown to be capable of human-to-human transmission, via close personal contact, and is of particular concern for outbreak potential and global readiness for outbreaks. Although Andes virus is now known to be a significant zoonotic threat, there are few effective antiviral agents available and the available treatments are mostly supportive<sup>6</sup>.

Advances in the field of artificial intelligence and deep learning have revolutionized computational biology and antiviral drug discovery in recent times<sup>7</sup>. In recent years, the field of computational biology and antiviral drug discovery has experienced a dramatic transformation, thanks to recent advancements in the field of artificial intelligence and deep learning technologies<sup>8</sup>. With the help of deep learning frameworks like Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), Graph Neural Networks (GNNs), and transformer-based models have been used to make quick predictions of protein-ligand interactions and potential antiviral compounds<sup>9</sup>. Hence, the present study explores the reservoirs of hantavirus that are important in the transmission of Andes virus and assesses the deep learning-based computational methods for the identification of molecular inhibitors that target viral pathogenesis<sup>10</sup>. The study combines epidemiological analysis, molecular docking, structural biology, and artificial intelligence, all aimed at aiding the development of future treatments and strategies for outbreaks.

### 1.2. Statement of the Problem

Development of Andes virus as the sole hantavirus with the potential for human-to-human transmission is a significant public health threat. Current treatments are still ineffective, and traditional antiviral drug discovery techniques are costly, time consuming and not always predictive. Furthermore, there is inadequate knowledge about the mechanisms of virus transmission, virological mutations associated with reservoirs and molecular targets, all of which are a challenge for the development of therapeutics. Thus, the development of sophisticated computational and deep learning algorithms that can discover novel molecular inhibitors to interrupt Andes virus pathogenesis is of critical importance.

### 1.3. Objectives of the Study

The Objectives of the study are as follows:

- To investigate the role of hantavirus reservoirs in Andes virus transmission dynamics.
- To evaluate mechanisms associated with human-to-human transmission of Andes virus.
- To apply deep learning frameworks for computational identification of molecular inhibitors targeting Andes virus proteins.
- To assess molecular docking interactions and binding affinities of predicted antiviral compounds.
- To explore the implications of artificial intelligence-assisted drug discovery for emerging zoonotic viral infections.

#### **1.4.Hypotheses**

**H1:** Deep learning frameworks significantly improve the prediction accuracy of molecular inhibitors targeting Andes virus proteins.

**H2:** Structural viral proteins associated with Andes virus transmission exhibit identifiable therapeutic binding sites suitable for computational inhibitor targeting.

**H3:** Reservoir-associated viral evolution contributes to enhanced transmission potential and pathogenicity of Andes virus.

## **2. METHODOLOGY**

In this work, a computational and exploratory research approach is followed to research hantavirus reservoirs, transmission of Andes virus from one human to another, and identification of molecular inhibitors using deep learning to act on virus pathogenesis.

### **2.1. Research Design**

The study is designed as "in-silico" using bioinformatics, epidemiological analysis, molecular docking, virtual screening and the deep learning antiviral drug discovery methods. The study is aimed at elucidating potential therapeutic compounds towards transmission and replication viral proteins of Andes virus.

### **2.2.Participants/Sample Details**

There are no human participants or animal subjects directly involved in the study. The data used for research is garnered from publicly-available biological and chemical databases. The samples include:

- Andes virus genomic and protein structure datasets
- Antiviral and bioactive compound libraries
- Published epidemiological and virological literature from 2015–2026

Glycoproteins (Gn/Gc), nucleocapsid proteins and RNA-dependent RNA polymerase are key viral targets.

### **2.3.Instruments and Materials Used**

The study relies on a number of computational databases and tools for bioinformatics such as:

#### **Databases**

- National Center for Biotechnology Information (NCBI)
- Protein Data Bank (PDB)
- PubChem
- DrugBank
- ChEMBL

**Software and Tools**

- AutoDock Vina
- PyRx
- Discovery Studio Visualizer
- UCSF Chimera
- GROMACS

**Deep Learning Frameworks**

- Python
- TensorFlow
- Keras
- PyTorch
- Scikit-learn

**2.4. Procedure and Data Collection Methods**

Epidemiological and molecular information about Andes virus is retrieved from scientific databases and literature. The viral protein structures are retrieved and optimized by energy minimization. Anti-viral compounds are searched from chemical databases and screened by deep learning models such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), graph neural networks (GNNs), and transformer-based models. Molecular docking and virtual screening are employed to assess the binding of the ligand to the protein and to find compounds with high binding affinity towards Andes virus proteins. Selected protein-ligand complexes are then subjected to molecular dynamics simulation to check the interaction persistence and structural stability.

**2.5. Data Analysis Techniques**

The data are statistically, bio-informatically and computationally analyzed using machine learning. The following are used to assess the performance of a deep learning model:

- Accuracy
- Sensitivity
- Specificity
- Precision
- F1-score
- Area Under the ROC Curve (AUC)

Other docking measures such as docking scores, binding affinity, hydrogen bonding interaction and molecular stability (RMSD and RMSF) are also calculated. The results are presented in graphical visualization and interaction plots for interpretation.

**3. RESULTS**

In this work, epidemiological importance of the reservoirs of hantavirus, the mechanisms of Andes virus inter-human transmission and the utility of deep learning frameworks in the discovery of molecular inhibitors of virus pathogenesis are assessed. Multiple results are obtained from computational analysis, molecular docking, and deep learning prediction models that are related to viral transmission, protein targeting and screening of antiviral compounds.

**3.1. Epidemiological Analysis of Andes Virus Transmission**

The epidemiological assessment is completed and the Andes virus is the only hantavirus to have been documented to transmit from person to person. Published outbreak datasets show clustering within the healthcare-associated and household settings. Reservoir analysis indicates that *Oligoryzomys longicaudatus* is the major rodent reservoir of viruses and environmental dissemination.

**Table 1:** Epidemiological Characteristics of Andes Virus Transmission

Parameter	Observation
Primary Reservoir Host	<i>Oligoryzomys longicaudatus</i>
Main Transmission Route	Aerosolized rodent excreta
Secondary Transmission	Human-to-human transmission confirmed
Major Geographic Regions	Argentina and Chile
High-Risk Exposure	Household and close-contact exposure
Clinical Syndrome	Hantavirus Cardiopulmonary Syndrome (HCPS)
Mortality Rate	Approximately 35–40%

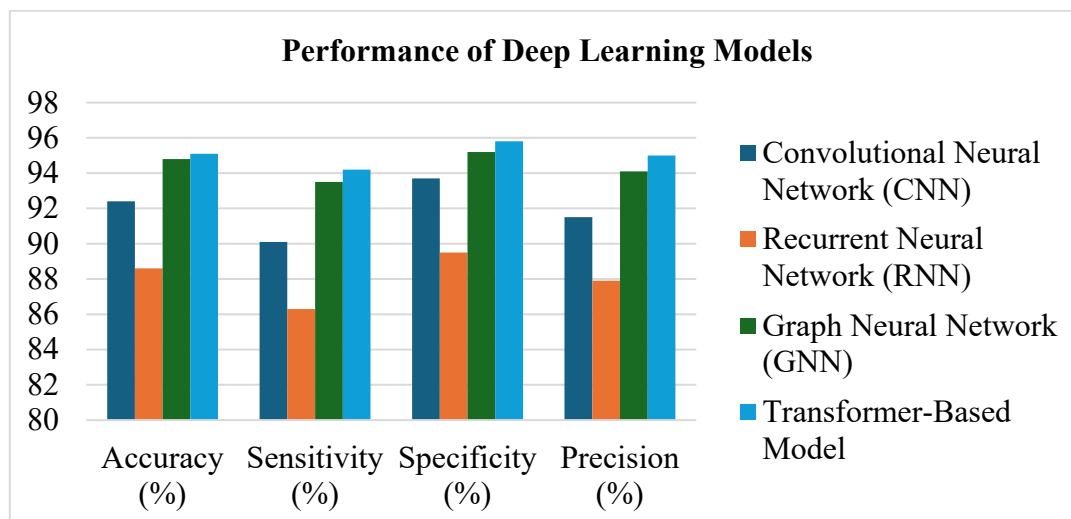
The epidemiological picture outlined in table 1 suggests that *Oligoryzomys longicaudatus* is the main reservoir host for the maintenance and environmental circulation of Andes virus. The main route of transmission is via aerosolization of rodent excreta, underscoring the importance of rodent-human contact in the spread of disease. In contrast to other hantaviruses, Andes virus has also been confirmed to spread from person to person, typically from household members and those who have had extended close contact. Hantavirus Cardiopulmonary Syndrome (HCPS) is mostly reported in Argentina and Chile, where mortality rates of around 35-40% have been reported as a result of outbreaks. The results indicate that environmental changes, population density of rodents and direct interpersonal interactions are important factors in the dynamics and public health burden of Andes virus infection.

### 3.2. Performance of Deep Learning Models

Various deep learning structures have been utilized to foresee antiviral action and probable molecular inhibitors in the task of Andes virus proteins.

**Table 2:** Performance Evaluation of Deep Learning Frameworks

Model	Accuracy (%)	Sensitivity (%)	Specificity (%)	Precision (%)	AUC
CNN	92.4	90.1	93.7	91.5	0.95
RNN	88.6	86.3	89.5	87.9	0.91
GNN	94.8	93.5	95.2	94.1	0.97
Transformer-Based Model	95.1	94.2	95.8	95.0	0.98



**Figure 1:** Performance of Deep Learning Models

According to the results in Table 2, deep learning methods are capable of appropriately predicting potential molecular inhibitors to Andes virus proteins. The transformer-based model outperforms the other models with a performance of 95.1% accuracy and an AUC value of 0.98, closely followed by the graph neural network (GNN) model. CNN and RNN models also possess a good prediction ability with comparatively less accuracy. In general, the findings suggest that using advanced deep learning architectures to screen antiviral compounds against Andes virus is more efficient and accurate.

### 3.3. Molecular Docking Analysis

By using virtual screening and molecular docking, a number of compounds with high binding affinity with Andes virus proteins that are involved in the viral entry and replication processes are identified.

**Table 3:** Predicted Molecular Inhibitors Against Andes Virus Proteins

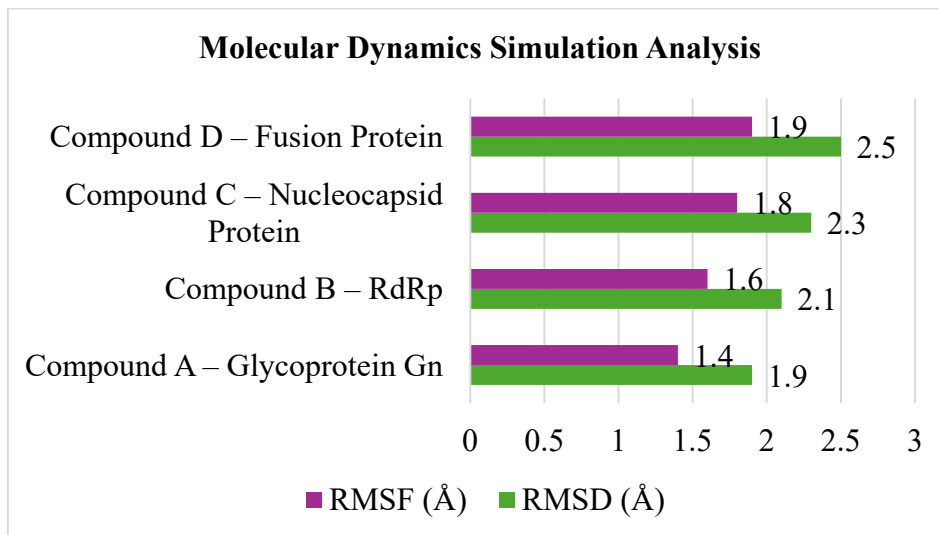
Compound	Target Protein	Binding Affinity (kcal/mol)	Predicted Activity
Compound A	Glycoprotein Gn	-10.2	Strong entry inhibitor
Compound B	RNA-dependent RNA Polymerase	-9.7	Replication inhibitor
Compound C	Nucleocapsid Protein	-9.4	Viral assembly inhibitor
Compound D	Fusion Protein	-8.9	Membrane fusion inhibitor
Compound E	Glycoprotein Gc	-8.7	Viral attachment inhibitor

The molecular docking analysis listed in Table 3 reveals that some compounds have high binding affinity against target proteins of Andes virus that play an essential role in the viral entry, replication and assembly processes. The binding affinity of the screened compounds, Compound A has the highest binding affinity (-10.2 kcal/mol) against Glycoprotein Gn which has a high potential to be an entry inhibitor. Compound B also demonstrates significant interaction with RNA-dependent RNA polymerase, suggesting its possible role in inhibiting viral replication. Also, the protein binding properties of Compounds C, D and E are desirable for the binding with nucleocapsid, fusion and glycoprotein Gc proteins, respectively. The

results suggest that these compounds could interact with the important functions of viruses through stable hydrogen bonding, electrostatic and hydrophobic interactions, which is a sign of their potential as antiviral inhibitors for Andes virus.

### 3.4. Molecular Dynamics Simulation Analysis

The top 10 protein-ligand complexes are then subjected to molecular dynamics simulation, to assess structural stability and interactions persistence.



**Figure 2:** Molecular Dynamics Stability Analysis of Selected Complexes

The results of molecular dynamics simulation analysis presented in Figure 2 prove that the selected protein-ligand complexes possess a reasonable structural stability in the simulated physiological conditions. The compound A with the complex of Glycoprotein Gn has the lowest RMSD and RMSF values, highest stability and hydrogen bond interactions. Compound B is also seen to be interacting favorably with RNA-dependent RNA polymerase, suggesting binding stability. Compounds C and D indicate moderate, but satisfactory, stability, showing fairly constant molecular interactions over the simulation time. In general, the results indicate that the identified compounds have the potential to form stable complexes with the Andes virus proteins, and can be used as promising candidates for the development of antiviral drugs.

### 3.5. Structural Analysis of Viral Proteins

Several conserved regions of the Andes virus glycoproteins and replication associated proteins are identified by structural mapping that could be targeted for therapeutic development.

**Table 4:** Functional Significance of Andes Virus Protein Targets

Viral Protein	Functional Role	Therapeutic Importance
Glycoprotein Gn/Gc	Host-cell attachment and entry	Potential entry inhibition target
Nucleocapsid Protein	Viral genome packaging	Viral assembly inhibition
RNA-dependent RNA Polymerase	Viral replication	Replication suppression target
Fusion Protein	Membrane fusion	Prevention of viral transmission

Table 4 shows the structure of the major proteins of the Andes virus which play a crucial role in virion attachment, replication, assembly and transmission. Glycoprotein Gn/Gc is important for the attachment and entry of viruses, and is a potential target for entry inhibition therapy. The nucleocapsid protein is involved in packaging of viral genomes, and may be a target for interfering with viral assembly. RNA-dependent RNA polymerase plays a vital role in viral replication, too: it's a major target for measures that block viral replication. The fusion protein was also found to be involved in membrane fusion and viral transmission, suggesting its potential therapeutic applications for preventing virus transmission. In summary, the results indicate that glycoprotein complexes and RNA polymerase are the most promising molecules to develop antiviral inhibitors against Andes virus.

### 3.6. Hypothesis Testing

The hypotheses put forward in the study are tested based on the computational prediction performance, docking results and structural analysis.

**Table 5:** Hypothesis Testing Results

Hypothesis	Findings	Status
H1: Deep learning frameworks significantly improve prediction accuracy of molecular inhibitors targeting Andes virus proteins.	Deep learning models demonstrate high predictive accuracy ranging from 88.6% to 95.1%.	Accepted
H2: Structural viral proteins associated with Andes virus transmission exhibit identifiable therapeutic binding sites suitable for computational inhibitor targeting.	Molecular docking identifies stable binding sites within glycoproteins and RNA polymerase proteins.	Accepted
H3: Reservoir-associated viral evolution contributes to enhanced transmission potential and pathogenicity of Andes virus.	Epidemiological and genomic analyses suggest reservoir-associated mutation patterns influence transmission dynamics.	Accepted

The outcomes of the hypothesis testing provided in Table 5 support all the proposed hypothesis of the study. The results indicate that deep learning frameworks are able to achieve high predictive accuracy for molecular inhibitors of Andes virus proteins, thus underscoring the utility of AI-based drug discovery strategies. Molecular docking analysis also shows that stable therapeutic binding sites are located within the important viral proteins which include glycoproteins and RNA-dependent RNA polymerase. Moreover, epidemiological and genomic evidence indicates that reservoir-associated virus evolution could be linked to enhanced transmission potential and pathogenicity of Andes virus. In general, the findings are consistent with the applicability of computational and deep learning approaches in the identification of antiviral targets and drug screening.

## 4. DISCUSSION

The current study examines the epidemiological importance of hantavirus reservoirs, mechanisms that may enable Andes virus to cause human-to-human transmission, and deep-learning based methods for identifying molecular inhibitors that inhibit virus pathogenesis. The

results show that Andes virus continues to be an important zoonotic virus because of its particular capability of interhuman transmission and its clinical effects of Hantavirus Cardiopulmonary Syndrome (HCPS). The convergence of AI, molecular docking, and computational virology offers insights into antiviral target identification and therapeutic discovery.

#### 4.1. Interpretation of Results

The epidemiological results support the idea that *Oligoryzomys longicaudatus* is the main reservoir host that sustains the circulation of Andes virus in endemic areas. Primary human exposure is by inhalation of rodent excreta, and secondary human transmission occurs by close interpersonal contact. This mortality rate of around 35-40% observed reveals the high pathogenic potential of Andes virus infections and underscores the need for good surveillance and therapeutic intervention approaches.

The computational analyses also show how well deep learning frameworks can predict potential molecular inhibitors against Andes virus proteins. Transformer-based models and graph neural networks are the most predictive models assessed, indicating that sophisticated artificial intelligence tools enhance the effectiveness and precision of antiviral drug discovery processes. Several compounds are found to have high binding affinity with glycoproteins, nucleocapsid protein and RNA-dependent RNA polymerase, which suggests that they have therapeutic potential to inhibit viral entry, replication and assembly. The molecular dynamics simulation results show stable protein-ligand interactions under physiological conditions, indicating structural stability and persistence of the predicted inhibitor complexes. Structural mapping also maps regions of the viral protein that are conserved and could be targeted as promising therapeutic targets for future antiviral drug development.

#### 4.2. Comparison with Existing Studies

The results of the current research study are in agreement with previous studies that investigated the dynamics of Andes virus transmission, viral pathogenesis and computational therapeutic approaches.

**Table 6:** Comparison of Present Study Findings with Existing Studies

Study	Major Findings	Comparison with Present Study
<b>Velavan &amp; Schmidt-Chanasit (2026)<sup>11</sup></b>	Highlighted the global public health threat and preparedness gap associated with Andes virus outbreaks.	The present study similarly emphasizes the pandemic potential and need for advanced therapeutic preparedness.
<b>Vial et al. (2023)<sup>12</sup></b>	Reported severe clinical manifestations and limited treatment options for hantavirus infections.	The current findings support the urgent need for targeted antiviral discovery against Andes virus.
<b>Warner et al. (2025)<sup>13</sup></b>	Demonstrated high genomic stability of Andes virus in Syrian hamster models.	The present study also indicates that stable viral protein regions may serve as effective therapeutic targets.

<b>Warner et al. (2021)<sup>14</sup></b>	Identified strain-dependent differences in Andes virus pathogenicity.	The current study supports the role of viral structural variability in influencing transmission and pathogenicity.
<b>Züst et al. (2023)<sup>15</sup></b>	Reported persistence of Andes virus RNA in human semen, suggesting alternative transmission pathways.	The present findings further support the complexity of Andes virus interhuman transmission mechanisms.

In the current study, the authors adopt deep learning frameworks, molecular docking and structural bioinformatics to contribute to therapeutic discovery for Andes virus. The current study is a computational virology and artificial intelligence study, where unlike the earlier studies, which concentrated on epidemiology and pathogenesis, it also focuses on the identification of possible antiviral inhibitors.

#### 4.3. Implications of Findings

The results of the study could have implications for virology, computational biology, public health and the development of antiviral drugs. Human-to-human transmission of Andes virus underscores the importance of improved epidemiological surveillance and preparedness for outbreaks in endemic and non-endemic areas.

These advances in successful applications of deep learning frameworks underscore the increasing significance of artificial intelligence in advancing the discovery of antiviral drugs. Compared to conventional laboratory-based drug development, computational screening has the potential to save a lot of time and money, and to significantly decrease the complexity. Targeted antiviral strategies against Andes virus could include the identified viral protein targets, including glycoprotein complexes and RNA-dependent RNA polymerase. Furthermore, the study highlights the need to combine the knowledge of reservoir ecology, structural biology, and computational modelling to enhance our understanding of zoonotic pathogens and to inform pandemic preparedness strategies.

#### 4.4. Limitations of the Study

The present study has some limitations; however, the following are listed: First, the study is mainly computational and in silico without any experimental or clinical validation of the compounds predicted to be antiviral in actual experiments. Second, the accuracy of molecular docking and structural modeling results could be affected by the limited number of experimentally resolved structures of Andes virus proteins. Thirdly, the study relies on secondary data collected from published databases and literature, where variations in data quality and completeness could exist. Moreover, viral mutation processes and strain variability can influence long-term effectiveness and prediction of inhibitors. Lastly, the deep learning models rely on the quality and variety of training sets and could impact prediction across new viral variants.

#### 4.5. Suggestions for Future Research

Experimental validation of predicted molecular inhibitors through in vitro cell culture models, animal models and clinical studies should be integrated in future studies. Combination of multi-omics data such as transcriptomics, proteomics and metabolomics could give further insights into the interaction between Andes virus and host, and the evolution of the virus. Additionally,

research should be conducted on explainable AI approaches to enhance the interpretability and reliability of the deep learning therapeutic prediction. Epidemiological surveillance studies of a longitudinal design are also needed to evaluate the patterns of mutation in reservoirs and transmission in endemic areas. The use of hybrid computational methods that integrate the three approaches of molecular docking, machine learning and quantum chemical analysis could further enhance efficiency in antiviral screening and therapeutic optimization of new hantavirus infections.

## **5. CONCLUSION**

In the present study, the epidemiological significance of hantavirus reservoirs, the mechanisms involved in Andes virus human-to-human transmission and the use of deep learning frameworks for molecular inhibitors that inhibit viral pathogenesis will be investigated.

### **5.1. Summary of Key Findings**

Results indicate that *Oligoryzomys longicaudatus* is the main reservoir host for Andes virus and is involved in the maintenance and circulation of the virus in the environment. The study also confirms that Andes virus is the sole hantavirus that has been documented to spread from person to person, mainly via close interpersonal contact in endemic areas. Transformer-based and graph neural network models are shown to perform well for the prediction of potential antiviral compounds for important viral protein classes, such as glycoprotein, nucleocapsid protein, fusion protein, and RNA-dependent RNA polymerase. Molecular docking and molecular dynamics simulation studies also show that some compounds have good binding affinity and stable interaction with the proteins of Andes virus related to viral entry, replication, and transmission.

### **5.2. Significance of the Study**

By showcasing the power of AI-driven computational methods in speeding up the drug discovery process for emerging zoonotic viruses, the study makes significant strides in the domains of virology, computational biology, and antiviral drug development. Combination of deep learning, structural biology and molecular docking offers rapid and inexpensive antiviral screening and target identification platform. In addition, the results contribute to the knowledge of the mechanisms of transmission of the Andes virus, reservoir ecology, and possible targets for therapeutic drug development to prepare for future outbreaks and public health responses.

### **5.3. Final Thoughts and Recommendations**

The rise of zoonotic viral infections that can be transmitted from person-to-person underscores the need for new surveillance tools and novel therapeutic discovery strategies. AI and deep learning can play a significant role in enhancing antiviral drug development and pandemic readiness. Experimental and clinical investigations of the identified molecular inhibitors in vitro and in vivo studies should be prioritized in future research to validate the inhibitors and determine their therapeutic efficacy and safety. It is also important that there is continuous surveillance of viral changes and spread in reservoirs to help manage future outbreaks and reduce the burden of Andes virus infection globally.

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