Article type: Editorial

Home Page URL: https://www.alliedacademies.org/virology-research/

Machine learning in antiviral drug discovery: Accelerating innovation.

Ualiveya Thuluva*

Department of Microbial Biotechnology, University of Oxford, UK

***Correspondence to:** Ualiveya Thuluva, Department of Pharmacy, University of Baghdad, Iraq, E-mail: ualiveya@stjude.org

Received: *04-Aug-2025, Manuscript No. AAVRJ-25-171356;* ***Editor assigned:*** *05-Aug-2025, PreQC No. AAVRJ-25-171356(PQ);* ***Reviewed:*** *19-Aug-2025, QC No. AAVRJ -25-171356;* ***Revised:*** *23-Aug-2025, Manuscript No. AAVRJ -23-171356(R);* ***Published:*** *30-Aug-2025, DOI:10.35841/aavrj-9.3.206*

Introduction

The emergence of viral pandemics such as COVID-19, Ebola, and Zika has underscored the urgent need for rapid and effective antiviral drug development. Traditional drug discovery pipelines are often slow, expensive, and labor-intensive, taking years to move from target identification to clinical approval. In recent years, machine learning (ML)—a subset of artificial intelligence (AI)—has revolutionized biomedical research by offering powerful tools to accelerate antiviral drug discovery. By analyzing vast datasets, predicting molecular interactions, and optimizing drug candidates, ML is reshaping how we respond to viral threats [1].

Machine learning algorithms can identify patterns and relationships in complex biological data that are difficult or impossible to detect using conventional methods. In antiviral drug discovery, ML is applied across multiple stages: ML models analyze genomic and proteomic data to pinpoint viral proteins or host factors essential for replication. ML predicts which molecules are likely to bind effectively to viral targets, reducing the need for exhaustive laboratory screening. ML can identify existing drugs with potential antiviral activity by comparing molecular structures and biological effects. ML helps refine drug candidates for potency, selectivity, and safety before clinical trials. These capabilities dramatically reduce time and cost, enabling faster responses to emerging viral threats [2].

Safety is paramount in drug development. ML algorithms predict absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties based on molecular features. This allows researchers to eliminate harmful compounds early in the pipeline. For example, deep learning models trained on toxicology databases can flag compounds likely to cause liver damage or cardiac arrhythmias. Integrating these predictions into antiviral development improves candidate selection and reduces late-stage failures. ML models require large, high-quality datasets. Incomplete or biased data can lead to inaccurate predictions. Complex models like deep neural networks often function as "black boxes," making it difficult to understand how decisions are made. Models trained on one virus may not perform well on others without retraining. ML predictions must be experimentally confirmed, requiring close collaboration between computational and experimental scientists. Identifying viable drug targets is a critical first step in antiviral development. ML models trained on viral genome sequences and protein structures can predict functional domains and interactions with host cells. For example, deep learning algorithms have been used to map the SARS-CoV-2 spike protein and its binding affinity to ACE2 receptors, guiding the development of entry inhibitors. ML also aids in identifying host factors that viruses exploit. By integrating transcriptomic and proteomic data, ML can reveal host pathways that support viral replication, offering alternative therapeutic targets [3].

Virtual screening involves evaluating thousands to millions of compounds for potential binding to a target protein. ML enhances this process by learning from known ligand-target interactions and predicting binding affinities with high accuracy. Algorithms such as random forests, support vector machines, and deep neural networks are commonly used. For instance, ML-driven docking tools like DeepDock and AtomNet have been employed to screen compounds against viral proteases, such as those in HIV and SARS-CoV-2. These tools

prioritize candidates for experimental validation, saving time and resources. Drug repurposing—finding new uses for approved drugs—is a cost-effective strategy, especially during outbreaks. ML models can analyze chemical structures, gene expression profiles, and clinical data to identify repurposing opportunities [4].

During the COVID-19 pandemic, ML helped identify drugs like remdesivir and baricitinib as potential treatments by comparing molecular fingerprints and disease signatures. Platforms such as BenevolentAI and DeepChem have demonstrated the power of ML in rapidly generating hypotheses for repurposed antivirals. Viruses mutate rapidly, often leading to drug resistance. ML can forecast resistance patterns by analyzing viral mutation data and predicting how changes affect drug binding. This is particularly useful for RNA viruses like influenza and HIV. ML models also simulate viral evolution under drug pressure, helping researchers design compounds less susceptible to resistance. These predictive capabilities are crucial for developing durable antiviral therapies [5].

Conclusion

Machine learning is accelerating innovation in antiviral drug discovery, offering tools to identify targets, screen compounds, predict resistance, and ensure safety. As viral threats evolve, so must our strategies. By harnessing ML's predictive power and integrating it with experimental science, we can build faster, smarter, and more resilient antiviral pipelines. The future of antiviral therapeutics lies not just in chemistry and biology—but in algorithms that learn, adapt, and innovate.

References

1. Timpe JM, Stamataki Z. Hepatitis C virus cell?cell transmission in hepatoma cells in the presence of neutralizing antibodies. Hepatology. 2008;47:17?24.
2. Rehermann B. Chronic infections with hepatotropic viruses: mechanisms of impairment of cellular immune responses. Semin Liver Dis. 2007;27:152?60.
3. Trucchi C, Orsi A. State of the art, unresolved issues, and future research directions in the fight against hepatitis C virus: perspectives for screening, diagnostics of resistances, and immunization. J Immunol Res. 2016;2016:1412840.
4. Vergniol J. Noninvasive tests for fibrosis and liver stiffness predict 5?year outcomes of patients with chronic hepatitis C. Gastroenterology. 2011;140:1970?79.
5. Zhong YW. IL28B SNP rs12979860 is the critical predictor for sustained viral response in Chinese children aged 1 to 6 years with chronic hepatitis C. Int J Biol Sci. 2016;12:1357-62.

Citation: Thuluva U. Machine learning in antiviral drug discovery: Accelerating innovation. Virol Res J. 2025;9(3):206