



Artificial Intelligence in Healthcare and Drug Discovery: From Predictive Diagnostics to Precision Medicine

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Abstract

The integration of artificial intelligence (AI) and deep learning with the biomedical research marks a critical inflection point, shifting the paradigm from addressing symptoms to predicting and acting at the molecular level. In many diagnostic models, the chain reaction triggered by a chronic infection is often overlooked. In this review, we examine the capability of AI models to unravel these complex dynamics within viral-host systems. By analyzing 39 key studies, we evaluate the application of novel computational methods in two major domains: advanced clinical diagnostics and de novo drug design.

Silently existing chronic conditions, such as chronic Hepatitis, can lead to immune exhaustion, leaving individuals more susceptible to secondary infections including SARS-CoV-2 (COVID-19) and Human Papillomavirus (HPV). For diagnostics, we focus on genomic surveillance, radiomics, and Explainable AI (XAI) for identifying multi-organ pathologies. For pharmacology, we examine the transformative role of generative models, including AlphaFold 3, HelixFold 3, and large foundational models (Evo 2, Geneformer, ESM-2). We discuss Graph Neural Networks (GraphDTA) and diffusion models in successfully identifying novel antimicrobial agents like Halicin and Abaucin. Finally, we explore clinical and regulatory barriers to the full integration of AI in mapping patient pathologies.

Keywords: Artificial Intelligence (AI), Healthcare, Drug Discovery, Precision Medicine, Machine Learning, Deep Learning, Protein Structure Prediction, AlphaFold 3, Graph Neural Networks (GNNs), Drug

Repurposing, Explainable Artificial Intelligence (XAI), Radiomics, Foundation Models, Biomedical Research.

1. Introduction

Artificial Intelligence (AI) is fundamentally restructuring modern healthcare by enabling researchers and clinicians to analyze massive, high-dimensional medical datasets, including electronic health records (EHRs), genomic sequences, and non-invasive radiomics.⁽²⁹⁾ By utilizing advanced machine learning and deep learning techniques AI identifies complex systemic patterns that are virtually impossible to detect through traditional clinical methods. This capability is changing the medical determinant from reactive symptom management to predictive analytics, where models use real-time patient report to estimate disease risk and support early intervention/prediction.

Furthermore, the integration of these predictive algorithms into Clinical Decision Support Systems (CDSS) requires overcoming the inherent "black box" nature of deep learning.⁽²⁶⁾ Explainable Artificial Intelligence (XAI) techniques, notably the SHAP (SHapley Additive exPlanations) framework are now essential to decode how models arrive at predictions, increasing diagnostic transparency and building the crucial clinical trust necessary to implement AI-assisted healthcare.⁽²⁷⁾

Beyond clinical diagnostics, AI is revolutionizing generative pharmacology by addressing the severe bottlenecks of conventional drug discovery—a process that notoriously requires an average investment of *US\$2.6 billion* over 10–15 years with a **90%** clinical attrition rate.⁽³¹⁾ Historically,

researchers relied heavily on traditional Computer - Aided Drug Design (CADD) and molecular docking to estimate how a small molecule binds

to a target protein based on basic molecular forces (e.g., hydrogen bonding and $\pi - \pi$ stacking).

However, modern computational approaches have evolved far beyond extensive experimental screening. Today, AI facilitates *de novo* drug design generating entirely new & optimized molecular structures from scratch—alongside highly accurate retrosynthesis and reaction prediction. By using modern structural architectures like AlphaFold 3⁽²⁾ and representing molecules as dynamic topological graphs via Graph Neural Networks (GraphDTA),⁽¹⁸⁾ AI directly predicts complex drug-target binding affinities, greatly reducing the experimental effort expended on compounds that ultimately fail.

The ultimate clinical test for these integrated AI diagnostic and pharmacological models lies in unwinding systemic pathogenesis, particularly intractable chronic viral infections. Hepatitis B (HBV), for example, remains a leading cause of global liver disease. While current therapeutics—such as entecavir (ETV) and pegylated interferon- α which, effectively suppress viral replication, they seldomly achieve a functional cure because as they cannot eliminate the covalently closed circular DNA (ccc-DNA) reservoirs hidden within hepatocytes.

Therefore, many individuals remain hidden for years, enduring a delayed diagnosis that allows continuous antigen exposure to induce a strong state of "Immune Exhaustion". Rather than outright destroying the immune system, this active suppression creates a highly tolerant biological environment, serving as a primary trigger for opportunistic secondary pathologies—including the catastrophic cytokine storms observed in SARS -CoV- 2 (COVID- 19) and the persistence of oncogenic Human Papillomavirus (HPV). Bridging AI diagnostics to map this exhaustive cascade and AI pharmacology to target hidden reservoirs like ccc-DNA, represents the frontier of precision medicine.

2. CONCEPTUAL FRAMEWORK

THEORETICAL FOUNDATION – 2.1

Following the establishment of how chronic viral reservoir alter the host's baseline, clinical focus shifts to advanced detection using deep learning networks that predict RNA virus– host interactions⁽¹¹⁾ and anticipate mutations before they evade immune detection.^(14,15) To integrate this complex "black box" models clinically, researchers utilize Explainable AI frameworks like *SHAP* (*SHapley Additive exPlanations*) — which build crucial trust by decoding predictions and scoring the exact biomarkers triggering clinical alarms. ⁽²⁷⁾ Concurrently, Federated Learning, a decentralized data approach, allows hospitals to securely train these diagnostic algorithms across diverse population without ever exposing sensitive patient records. ⁽²⁸⁾

Once these diagnostic networks map a patient's systemic vulnerabilities, the computational focus

seamlessly transition to designing targeted therapeutics. Moving further the limitations of traditional molecular docking, the pharmaceutical frontier now uses deep learning approach like the Neurodock framework,⁽³⁹⁾ which upgrades static algorithms with neural networks to predict complex drug-target binding affinities with Translational Speed. Consequently, the field is undergoing a massive transition from simply screening existing drugs to utilizing Generative AI for *de novo* drug discovery,⁽³¹⁾ a pattern that builds entirely new therapeutic molecules from beginning.

To drive this generative paradigm - *Large Language Models (LLMs)* for Molecular Biology treat amino acid sequences as a decipherable language, learning the evolutionary "grammar" of proteins to generate entirely novel, functional enzymes ^(21,25)

Simultaneously Geometric Diffusion Models operate in a mathematical "latent space " to generate chemically valid , three-dimensional molecular structures while preserving strict 3D spatial geometry, ensuring the new drug perfectly fits a pathogen's active site.⁽³²⁾ Pushing these capabilities further, hybrid Quantum Computing algorithms, such as the Variational Quantum Eigensolver (VQE), are being explored to estimate ground-state molecular energies, promising unparalleled precision in calculating complex drug-target interactions . ⁽³⁴⁾

Eventually these advanced computational methods are deployed to untangle the web of chronic pathogenesis utilizing machine learning to rapidly screen millions of molecular graphs for

novel antimicrobial discoveries.^(9,10) Deep learning surveillance is strictly necessary to map the silent progression of diseases like Hepatitis, which subtly induces a profound state of immune exhaustion. Once this permissive baseline is identified then generative architectures engineer exact 3D molecules designed to clear hidden viral reservoirs - such as HBV ccc- DNA— that traditional drugs leave behind. Because this Hepatitis- induced exhaustion leaves patients highly susceptible to opportunistic infections, these AI - driven pipelines remain vital for protecting vulnerable patients against multi drug-resistant bacteria and catastrophic secondary viral storms triggered by SARS- CoV-2 (COVID- 19) or oncogenic HPV, setting a functional framework for the deployment of specialized AI models.⁽²³⁾

WORKING MODELS AND TRAINING – 2.2

- Developed by DeepMind, AlphaFold replaces slow, traditional methods like X-ray crystallography with deep learning to rapidly map the 3D shapes of cellular and viral proteins.⁽¹⁾
- **AlphaFold 1 & 2 (Protein Folding):**⁽¹⁾ Utilized evolutionary data to predict individual protein structures for rapid target identification.

AlphaFold 3 (Biomolecular Complexes) Upgraded to a generative, diffusion-based model to map interactions between proteins, DNA, RNA, and drug ligands.^(2,3) Researchers note the ongoing need to map alternative folds and account for structural binding spots.⁽⁵⁾

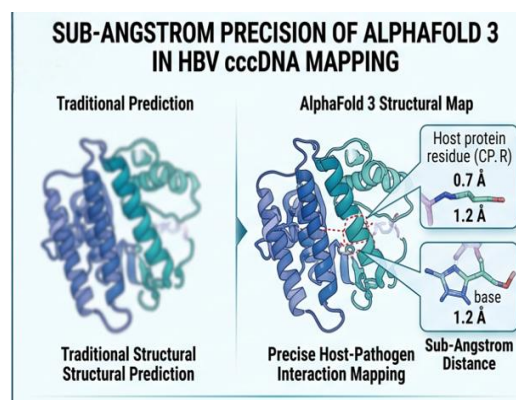


Figure 1

By iteratively denoising randomized atomic coordinates, AlphaFold 3 achieves **atomic-scale precision**. This enables precise mapping of how novel therapeutics bind directly to the intractable HBV ccc-DNA reservoir, accelerating the development of specialized drugs designed to clear chronic infections and reverse systemic immune exhaustion.

2.2.2. GeoLDM (Geometric Latent Diffusion Model)

GeoLDM is a generative AI model introduced in 2023 to generate realistic 3D molecular structures.⁽³²⁾ It combines diffusion models with geometric deep learning to produce chemically valid molecules while preserving molecular geometry.

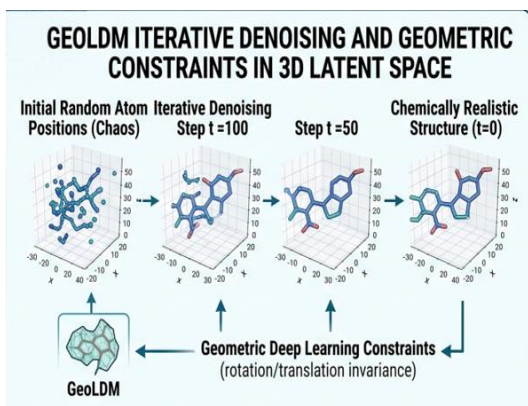


Figure 2:

It computationally designs small-molecule drugs with exact 3D precision before lab testing. For this study, this allows researchers to rapidly generate custom therapeutics that perfectly fit into complex viral reservoirs like HBV ccc-DNA, accelerating treatments designed to clear chronic infections and reverse immune exhaustion.

2.2.3. GraphDTA

Developed by Deakin University, GraphDTA utilizes graph neural networks to predict drug–target binding affinity using structural molecular graphs.⁽¹⁸⁾

- **GCN:** Learns structural features directly from molecular graphs.
- **GAT:** Uses attention mechanisms to identify critical neighbouring atoms.
- **GIN:** Captures highly complex molecular structures with high expressive power.

GraphDTA maps drugs as graphs alongside protein sequences to accurately predict binding

strength before lab testing. This allows researchers to rapidly screen candidate molecules that bind tightly to persistent viral targets, accelerating the clearance of chronic reservoirs to reverse systemic immune exhaustion.

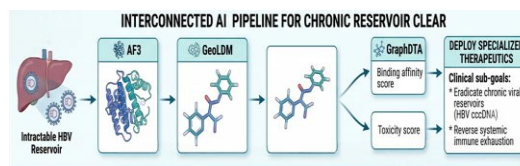


Figure 3

2.2.4. TxGNN

TxGNN leverages biomedical knowledge graphs and graph neural networks to identify new therapeutic uses for existing approved drugs.⁽²⁰⁾

- **KG Encoder:** Maps complex relationships among diverse biological entities.⁽¹³⁾
- **GNN Core:** Models explicit interactions between drugs, diseases, genes, and proteins.
- **TxGNN Explainer:** Decodes predictions by identifying the specific biological pathways driving them.

TxGNN reveals hidden drug-disease relationships to quickly identify approved medications for new uses. This helps researchers shorten development time by finding existing treatments that target chronic viral reservoirs or control secondary infections while reducing immune exhaustion.

2.2.5. Graph Neural Networks (GNNs)

GNNs map molecular structures as graphs — representing atoms as nodes and bonds as edges to learn chemical properties directly.^(12,17)

- **GCN:** Gathers features from adjacent atomic neighborhoods.⁽¹⁶⁾
- **GAT:** Employs attention mechanisms to weight the most critical neighboring atoms.
- **MPNN:** Passes information along chemical bonds to predict molecular behavior.

By predicting drug target interactions and toxicity from structural data - GNNs improve selection of promising drug candidates against chronic viral infections. This speeds development of safe high affinity therapies targeting persistent HBV ccc-DNA reservoirs while restoring weakened immune responses.

2.2.6. Evolutionary Scale Modeling (ESM)

Evolutionary Scale Modeling (ESM) is a family of transformer-based protein language models developed by *Meta AI* to understand proteins directly from their amino acid sequences.⁽²²⁾ ESM learns the "*language of proteins*" by analyzing millions of naturally occurring protein sequences without requiring labeled data.

Versions:

- **ESM-1v:** It is used for predicting the effects of amino acid mutations and identifying potentially harmful variants associated with diseases.
- **MSA Transformer:** (Multiple Sequence Alignment Transformer): analyzes

multiple sequence alignments to capture evolutionary conservation and improve predictions of residue contacts and protein structure.

- **ESM-IF1 (Inverse Folding Model):** It works in the opposite direction by designing amino acid sequences that can fold into a desired three-dimensional structure, making it highly valuable for protein engineering and de novo protein design.
- **ESM-2** - (model provides high-quality protein representations, while *ESMFold* predicts accurate three-dimensional protein structures directly from a single amino acid sequence without relying on multiple sequence alignments, making structure prediction much faster.

Together, these models have made ESM one of the most powerful AI platforms in computational biology, enabling rapid protein structure prediction, functional annotation, mutation analysis, and the design of novel therapeutic proteins.

2.2.7. ProGen

Developed by Madani et al., ProGen is a transformer-based Large Language Model (LLM) trained on 280 million sequences to learn the evolutionary patterns of natural proteins.^(21,25)

- **ProGen 1:** Generates and fine-tunes sequences that closely mirror the structure and function of naturally occurring proteins.

- *ProGen 2*: Generates entirely novel, *de novo* protein sequences that do not exist in nature.

ProGen treats amino acids as a decipherable biological language to rapidly accelerate protein engineering. This enables the highly efficient design of custom enzymes and novel biological therapeutics for advanced drug development, bypassing the slow timelines of traditional synthetic biology.

2.2.8. Evo

Developed by the Arc Institute and Stanford, Evo is a long-context genomic foundation model that learns the evolutionary "language" of biology by training directly on trillions of nucleotides from whole genomes across all domains of life. ⁽²⁴⁾

Models:

- Evo 1: Trained on prokaryotic and phage genomes to predict and generate DNA, RNA, and proteins simultaneously.
- Evo 2: Scaled to 40 billion parameters with a 1-million-token context window, expanding its training to include complex eukaryotic genomes, including human data.
- De Novo Systems (e.g., EvoCas9-1): Generates entirely novel, fully functional biomolecular machines, such as previously unknown CRISPR systems, from scratch

Evo predicts disease-causing genetic mutations at single-nucleotide resolution and co-designs custom protein-RNA systems, accelerating gene-

editing therapies and countering viral genetic drift.

2.2.9. Neurodock

Mechanism: Deep learning docking framework evaluating dynamic drug-target binding interactions. ⁽³⁹⁾

Replaces static docking to rapidly refine high-affinity drug candidates.

2.2.10. RegFormer

RegFormer is a foundation model developed to improve the analysis of single-cell RNA sequencing (scRNA-seq) data by integrating gene regulatory network information with gene expression data.

It is to identify important cellular features and better understand the complex relationships that control gene expression. ⁽¹⁹⁾

According to studies RegFormer could become a valuable tool for functional genomics, disease research, drug discovery, and precision medicine by providing a more comprehensive understanding of cellular behavior.

Model & Origin	Work (Core Mechanism / Function)	Uses (Assumed Applications in Various Diseases)
AlphaFold 2-3 (DeepMind)	Uses diffusion-based deep learning and iterative denoising to predict precise 3D biomolecular structures and complexes (proteins, DNA, RNA, ligands) from	Maps the precise structure of intractable viral targets (like HIV ccdNA) and host-pathogen interactions to identify vulnerabilities for targeted drug design.
HeliFold (Academic / Deep Learning Community)	Predicts complex 3D structures and folding patterns specifically focused on intricate biological molecules and RNA frameworks.	Maps the hidden structural configurations of viral RNA, aiding in the discovery of novel drug targets for RNA-based viruses and respiratory diseases.
GeoLM (Academic Research, 2023)	Employs geometric latent diffusion and geometric deep learning to generate chemically valid, 3D molecular structures while preserving exact spatial geometry.	Designs custom, <i>de novo</i> small-molecule therapeutics computationally tailored to perfectly fit into the active sites of chronic infections and therapy-resistant
GraphGAT (Duke University)	Utilizes Graph Neural Networks (GCN, GAT, GIN) to predict drug-target binding affinity by representing drugs as structural molecular graphs.	Screens millions of generated molecules to find candidates that bind tightly to persistent viral targets, ensuring high efficacy against chronic reservoirs.
TaGNN (Harvard University)	Uses biomedical knowledge graphs and graph neural networks to map and explore therapeutic relationships between drugs, diseases, and genes.	Facilitates zero-shot drug repurposing, identifying existing FDA-approved medications capable of alleviating immune exhaustion or treating diseases with no current therapies.
General GNNs (Deep Learning Community)	Learns expressive molecular representations by passing information between connected atoms (nodes) and chemical bonds (edges).	Predicts molecular properties, toxicity, and pharmacokinetics, optimizing the safety profile of candidate drugs for highly fragile, immunocompromised
ESM (e.g., ESM-2) (Meta AI)	Functions as a protein language model, treating amino acid sequences as a decipherable evolutionary "grammar" to generate novel proteins.	Engineers completely novel, functional enzymes and antimicrobial peptides designed to combat secondary opportunistic infections and multi-drug resistant bacteria.
Evo (Arc Institute / Stanford)	A genomic foundation model trained on millions of genomes to predict and design functional sequences across DNA, RNA, and proteins.	Predicts disease-causing genetic mutations and codesigns protein-RNA systems to anticipate and counter viral genetic drift.

Figure 4

(1,2,3,4,5,13,17,22,32,34)

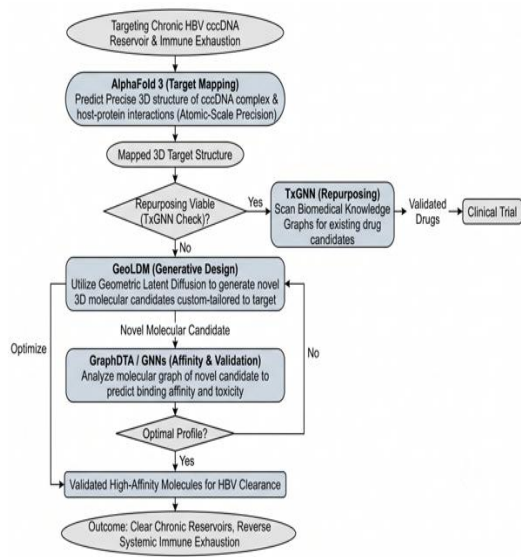


Figure 5

3. Critical Analysis

3.1 How the Our Theory and AI Models Correlates.

A careful review of current research shows that AI must combine real-time pandemic tracking, safe diagnostic tools, and clear decision-making to be effective. In their study on pandemic preparedness, *Baker and colleagues* proved that computational models should do more than track current outbreaks—they must predict how viruses mutate and spread over time.⁽³⁵⁾ Complementing this macro-level

Tracking, recent progress in *Advanced AI Liver Disorder Detection* shows how neural networks can catch subtle liver damage blood vessel

changes and early fibrosis long before severe liver failure happens.⁽³⁷⁾

If a patient's liver is already damaged AI would help doctors separate drug induced liver injury from a hepatitis flare up, lowering the risk of incorrect diagnosis and improving patient safety. However, before these tools are widely used in hospitals, they must be clear so doctors can understand, trust and confidently apply their predictions in clinical practice every day.⁽²⁶⁾

Bringing these different research areas together into one clear system requires connecting specialized AI tools:

- *Genomic Tracking:* Long-context models like *Evo*⁽²⁴⁾ and *ESM-2*⁽²²⁾ read genetic sequences to spot mutations in Hepatitis B/C and SARS-CoV-2 early, expanding the prediction goals of *Baker et al.*⁽³⁵⁾
- *3D Target Mapping:* When new viral variants emerge, *AlphaFold 3* creates high resolution 3D models of complex target structures, such as the HBV cccDNA host-protein configuration.⁽²⁾
- *New Molecule Design & Safety Screening:* *GeoLDM* designs novel small molecules made to suppress viral targets.⁽³²⁾ While *TxGNN* scans existing medical databases to find existing non – toxic drugs that can be repurposed.⁽²⁰⁾ *GraphDTA* tests these prospects against molecular models to verify strong affinity⁽¹⁸⁾ and enforces the safety rules & regulations set by *The Systematic AI DILI Review*.⁽³⁸⁾

- *Clear Explanations:* Explainable AI tools like SHAP turns complexed neural network predictions into a simple biological explanations,⁽²⁷⁾ fulfilling the clinical trust requirements/ criteria from “*The HCC AI Ethics Framework*”.⁽³⁶⁾

3.2 The Link Between Hepatitis and COVID-19

Examining the relationship between viral hepatitis and COVID-19 shows how a chronic liver disease and an acute respiratory infection can aggravate each other. People living with chronic hepatitis B or C often have ongoing low-grade inflammation in the liver, which gradually debilitates the immune system by reducing the effectiveness of T cells. When SARS-CoV-2 infects these patients, it can enter liver cells through ACE2 and TMPRSS2 receptors, leading to additional liver damage on top of the existing disease. Advanced AI-based liver diagnostic models can help monitor these changes and identify liver injury at an early stage.⁽³⁷⁾

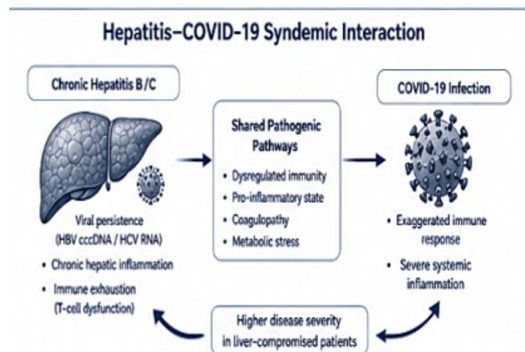


Figure 6

Since the liver plays a major role in metabolism and immune regulation, acute liver injury can reduce its ability to produce important protective

proteins and natural interferons. This weakens the body's antiviral response and allows SARS-CoV-2 to multiply more easily. At the same time, the intense inflammatory response associated with COVID-19 may revive inactive hepatitis B virus (HBV) ccc-DNA within liver cells, further worsening the patient's condition and health. These findings highlight that chronic hepatitis is more than just a liver disorder, as it can significantly increase the risk of severe illness during viral infections such as COVID-19.

3.3 Busting Medical Myths and Finding Future Cures

Analyzing this multi-model AI pipeline helps clear up three major clinical misconceptions:

1. *The Isolated Organ Myth:* It disproves the belief that viruses only affect one organ at a time, showing instead that immune system exhaustion links liver, lung, and cancer-related conditions together.⁽¹³⁾
2. *The Incurable Reservoir Myth:* It challenges the idea that hidden viral reservoirs like HBV cccDNA can never be destroyed, showing how generative diffusion models can design drugs specifically built to break apart these hidden targets.⁽³²⁾
3. *The Trial-and-Error Safety Risk:* It eliminates dangerous trial-and-error drug testing by using computers to screen out liver-toxic drug candidates before they are ever made in a lab, following the safety guidelines of *The*

Beyond hepatitis and COVID- 19, this connected approach offers a reusable mapping for tackling other persistent viruses. For example, with the *Human Papillomavirus (HPV)*, *Evo* can track genetic mutations ⁽²⁴⁾ while *AlphaFold 3* maps the 3D shapes of cancer-causing viral proteins (E6 / E7).⁽²⁾ Generative AI flow can then design targeted treatments capable of clearing hidden viral reservoirs, resetting immune function, and curing complex conditions across the whole body.

4. Challenges and Opportunities

4.1 Main Challenges

- *High Costs and Resource Limits:* Advanced AI models require expensive GPU clusters and immense electrical power, creating high financial barriers.
- *Accuracy and "Hallucinations":* AI can produce false target predictions or biologically impossible molecules that fail in physical laboratory testing. ⁽⁵⁾
- *Biological Complexity:* Static 3D models struggle to simulate dynamics, live cellular environments, and shift viral targets like HBV ccc-DNA.
- *Regulatory and Safety Risks:* Opaque "Black-Box" algorithms pose severe clinical risks if they lead to error in diagnoses (e.g., confusing drug toxicity with viral flares). ^(26,36)
- *Data Bias and Privacy:* Using patient health records carries security risks, while datasets biased toward high-

income populations lead to unequal global healthcare outcomes. ⁽²⁸⁾

4.2 In-Depth Analysis of Systemic Challenges

After all generative AI and foundation models have shown great promise in disease diagnosis, drug discovery, and disease surveillance, several practical challenges still limit their routine use in clinical settings.

- *Financial and Infrastructure Requirements:* Training and deploying large AI models with billions of parameters require advanced computing resources including high-performance GPUs, cloud platforms, and substantial energy consumption. The associated costs can be difficult for many healthcare organizations and research institutions to afford, particularly in low- and middle-income countries where viral hepatitis remains a major public health concern.
- *Accuracy Limitations and the Wet-Lab Gap:* Predictions generated through computational methods (in silico) do not always translate into successful biological outcomes (in- vivo). AI models may identify molecules that appear promising computationally but later show poor pharmacokinetic properties, unexpected toxicity, or limited stability during laboratory and clinical testing. As a result, extensive experimental validation remains an essential and time-consuming step in the drug development process. ⁽³¹⁾

- **Regulatory and Ethical Challenges:** Before AI-based diagnostic systems or AI-designed therapeutics can be introduced into clinical practice, they must meet strict regulatory and ethical standards. As highlighted in the Hepatocellular Carcinoma AI Ethics Framework,⁽³⁶⁾ regulatory agencies require evidence of safety, reliability, and transparency. Deep learning models that function as "black boxes" remain a concern because unclear decision-making processes could lead to serious clinical errors, such as confusing drug-induced liver injury (DILI) with acute viral hepatitis.⁽³⁸⁾
- **Data Bias and Global Health Inequalities:** Many AI models are trained primarily on genomic and clinical datasets collected from high-income countries. This imbalance may reduce prediction accuracy for populations that are underrepresented in these datasets. Expanding access to diverse and globally representative clinical data will be important to ensure that AI benefits patients across different geographical regions rather than increasing existing healthcare disparities.

5.1 Key AI Opportunities

- **Cost Reduction & Accessibility:** Open-source architectures,⁽²³⁾ model distillation and energy-efficient neural networks are actively lowering hardware entry points for global institutions.

- **Hybrid Physics & Automated Validation:** Combining physics-informed neural networks (PINNs) with automated wet-lab robotics allows real-time physical testing of AI-designed molecules.⁽³³⁾
- **Dynamic Cellular Simulation:** Integrating time-resolved molecular dynamics with multi-omic data enables AI to simulate live biological interactions beyond static 3D snapshots, acting as a digital twin for prescription medicines.⁽³⁰⁾
- **Transparent & Ethical AI:** Explainable AI (XAI) frameworks like SHAP decode deep learning predictions, delivering biological justifications that satisfy regulatory bodies and build clinician trust.⁽²⁷⁾
- **Equitable Global Data:** Privacy-preserving federated learning⁽²⁸⁾ and synthetic data generation allow models to train securely on diverse global populations without compromising patient privacy.

6. Discussion

Despite present obstacles, the course of computational medicine is preceding forward at the phenomenal pace. The technical constraints of today are fueling at rapid innovation across automated robotics, prototype distillation, and open-access research. As Explainable AI frameworks bring transparency to complex neural networks, clinician skepticism is steadily eroding.

By uniting long-context genomic surveillance, generative structural design, and rigorous safety guardrails, we are entering a transformative era of medicine. AI is no longer only a tool for reacting to health crises after they occur—it is becoming a proactive defence mechanism capable of predicting viral mutations, designing hepato-safe therapeutics, and breaking down deep rooted viral reservoirs before outbreaks intensifies. As these technology channels progress and becomes globally accessible, the dream of eliminating chronic co-occurring diseases like viral hepatitis and COVID-19 is rapidly evolving into a concrete biological reality.

7. Conclusion

Present data overwhelmingly confirms that the surging global weight of chronic viral hepatitis alongside stubborn viral threats like COVID-19 dictates an urgent public health imperative demanding a unified *AI framework*. By merging genomic surveillance (Evo, ESM-2), 3D target mapping (AlphaFold - 3), and generative drug discovery (GeoLDM, TxGNN, GraphDTA), our architecture attacks the interconnected health crisis feedback loop, wherein chronic hepatic inflammation and T-cell exhaustion worsen systemic viral disease mechanism.

Looking around in literature spanning pandemic preparedness (Baker et al.), liver diagnostics, DILI safety, plus Explainable AI ethics (SHAP), this flow shatters the myth of organ-isolated infections whilst computationally engineering liver-safe therapeutics. Acknowledging hurdles in-compute costs, model hallucinations or dataset bias, breakthroughs in model distillation and federated learning create a realistic path onward.

Finally, extending this multi-omic methodology toward other persistent microbes, like the Human Papillomavirus (HPV), shifts reactive healthcare toward a proactive, generative shield for global disease elimination.

8. Author Contributions

Abhijeet Pintu Goad: Conceptualization, Methodology, Principal Investigation, and Writing – Lead Draft Preparation.

Rohit Shamsundar Tawade: Project Administration, Data Curation, Formal Formatting, and Writing – Review & Editing.

Maryston Gregory Sequeira: Validation, Secondary Researcher, and Writing – Lead Reviewer.

Dr. Anupam Kumar: Supervision and Mentorship.

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39. June 1, 2026 | NEURODOCK: DEEP LEARNING APPROACHES IN MOLECULAR DOCKING AND DRUG DESIGN. *1Sukirti Yadav, 2Saumya Singh, 3Vaibhav Vishnoi, 4Mo Asad, 5Dr. Hari Krishna Yadav, 6Dr. Prashant Kumar Katiyar.