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Role of Artificial Intelligence in Drug Discovery and Repurposing: A Comprehensive Review

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ABSTRACT

Drug discovery is one of the most resource-intensive endeavours in modern science, requiring over 12 years and USD 2.6 billion on average to bring a single drug to market, with a clinical failure rate exceeding 90%. Artificial Intelligence (AI) is fundamentally transforming this process. This review examines how AI technologies — including machine learning, deep learning, graph neural networks, generative models, and natural language processing — are being applied across every stage of the drug discovery pipeline, with particular focus on drug repurposing. Key real-world case studies are analysed, including DeepMind's AlphaFold2, which predicted over 200 million protein structures; Insilico Medicine's AI-designed pulmonary fibrosis candidate developed in approximately 30 months; and BenevolentAI's identification of baricitinib as an FDA-approved COVID-19 treatment. Advantages including accelerated timelines and improved molecular design are considered alongside persistent limitations in data quality, model interpretability, and regulatory frameworks. The review concludes with implications for pharmacy education and future directions including foundation models, multimodal AI, and quantum-enhanced simulation.

Keywords: Artificial Intelligence, Drug Discovery, Drug Repurposing, Machine Learning, Deep Learning, Generative AI

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INTRODUCTION

Imagine you are searching for a single key that can open a very specific lock — but there are over one trillion possible keys to try. This is roughly what drug discovery feels like. Scientists are searching for molecules that can interact precisely with biological targets inside the human body, out of an almost unimaginably large chemical universe. The traditional approach to this problem has always relied on physical experiments, human expertise, and time — enormous amounts of time.

The numbers tell a difficult story. According to the Tufts Center for the Study of Drug Development, bringing a single drug from the laboratory to a patient's hands costs an average of USD 2.6 billion and takes 12 to 15 years. [1] Despite this investment, more than 90% of all drug candidates that enter clinical trials ultimately fail — most often because they turn out to be ineffective or toxic in ways that earlier testing did not predict. [2]

This is not a failure of science — it is a failure of scale. The challenge is that human biology is extraordinarily complex. The human body contains approximately 20,000 proteins, and the space of possible drug-like molecules that could interact with them has been estimated to exceed 10^{60} compounds. [3] No team of scientists, however talented or hardworking, can manually navigate a space that large.

Artificial Intelligence (AI) changes this equation fundamentally. AI systems — particularly those built on machine learning and deep learning — can learn patterns from vast biological and chemical datasets, make predictions about molecules they have never seen before, and even generate entirely new molecular structures optimized for therapeutic activity. What once took years can now take months; what once required a laboratory can now begin on a computer.

Among the most promising applications of AI is drug repurposing: the process of finding new therapeutic uses for drugs that are already approved and have established safety records in humans. Since the safety hurdle has already been cleared, AI-powered repurposing can deliver new treatments to patients in a fraction of the time required for entirely new drug development. The COVID-19 pandemic showed the world just how powerful this approach can be. [4]

This review provides pharmacy students, researchers, and healthcare professionals with a clear, evidence-based understanding of how AI is reshaping drug discovery — covering the tools and techniques involved, the real-world case studies that prove it works, and an honest assessment of the limitations that still need to be overcome.

THE TRADITIONAL DRUG DISCOVERY PROCESS: WHY IT NEEDS HELP

To understand what AI brings to drug discovery, we first need to appreciate why the traditional process is so difficult. Drug development follows a well-established pipeline — but each stage introduces serious bottlenecks that slow everything down.

The journey begins with target identification: finding the specific protein, enzyme, or receptor that is responsible for causing a disease. This alone can take years, because most diseases involve complex networks of biological interactions rather than a single clear culprit. Once a target is found, it must be validated — scientists must confirm that modifying this target will actually improve patient outcomes without causing harm elsewhere in the body [5].

The next stage, hit and lead discovery, involves testing thousands or millions of chemical compounds to find ones that interact with the target in a useful way. High-throughput screening (HTS) can test hundreds of thousands of compounds per day using robotic systems — but even this impressive rate barely scratches the surface of the available chemical space. The 'hits' that emerge from screening must then go through lead optimization — a process of chemical refinement that can take several more years. [6]

Only after all this work does a candidate enter preclinical testing (in cell cultures and animal models) and then clinical trials in three phases. Each phase adds years and millions of dollars — and the candidate can still fail at any point. An observation called 'Eroom's Law' has captured this uncomfortable reality: while computing power doubles roughly every two years (Moore's Law), drug discovery has historically become more expensive and less productive over time, not less. [7] AI is widely seen as the most promising answer to this paradox.

HOW ARTIFICIAL INTELLIGENCE WORKS IN DRUG DISCOVERY

Finding the Right Target

AI helps scientists identify which biological targets are most relevant to a given disease by analyzing massive datasets — genomic sequences, protein interaction networks, patient records, and published research — all at once. Machine learning models can detect subtle patterns across these data types that human analysis would miss, prioritizing targets that are both biologically meaningful and realistically 'druggable'. [8]

Graph Neural Networks (GNNs) have shown particular promise here, as they can model the complex web of protein-protein and gene-gene interactions that characterize biological systems. A 2020 study published in Cell used a deep learning model to screen over 100 million molecules and discovered Halicin — a novel antibiotic with activity against drug-resistant bacteria — entirely from computational screening. [9]

Virtual Screening: Testing Billions of Compounds Digitally

Instead of physically testing compounds in a laboratory, AI-powered virtual screening builds computational models that predict how well a molecule will bind to the target protein — based on the molecule's chemical structure alone. Modern deep learning models can evaluate billions of compounds in the time it takes traditional HTS to screen a few hundred thousand, at a fraction of the cost. [10]

This is not just a matter of speed — AI models can evaluate structural features and interaction energies with a level of nuance that earlier rule-based methods could not achieve. Libraries such as ZINC and ChEMBL, which contain tens of millions of real and commercially available compounds, serve as the starting point for many AI-driven screening campaigns.

Molecular Docking: How Does the Drug Fit?

Once promising candidates are identified through virtual screening, molecular docking simulates the physical interaction between the drug molecule and the target protein — predicting the exact geometry and binding energy of the drug-protein complex. The famous analogy of a key fitting into a lock is apt: not just any molecule that 'fits' will work; the fit must be precise, stable, and energetically favourable. [11].

AI improves molecular docking by enhancing the scoring functions used to rank binding poses, and by incorporating protein flexibility — the ability of a protein to change shape slightly when a drug binds — which traditional rigid docking algorithms cannot handle well.

ADMET Prediction: Will the Drug Be Safe?

One of the most common reasons drugs fail in clinical trials is not that they stop working against their target, but that they cause unexpected harm. ADMET — which stands for Absorption, Distribution, Metabolism, Excretion, and Toxicity — describes how a drug behaves inside the human body from the moment it is taken to the moment it is eliminated. [12]

AI tools such as SwissADME, pkCSM, and DeepTox can predict ADMET profiles from molecular structure alone — flagging problematic compounds before they ever reach a laboratory. DeepTox, a deep learning model developed for the Tox21 Data Challenge, outperformed all competing methods in predicting the toxicity of over 10,000 compounds across 12 different toxicity endpoints. [13]

Generative AI: Designing New Drugs from Scratch

Perhaps the most exciting frontier in AI-driven drug discovery is the use of generative models to design entirely new drug molecules — ones that do not exist in any existing library. Using architectures such as Variational Autoencoders (VAEs), Generative Adversarial Networks

(GANs), and transformer-based models, AI can explore chemical space proactively, generating novel molecular structures optimized for binding affinity, drug-likeness, and low toxicity. [14]

This approach transforms drug discovery from a search problem into a design problem — and the results have been striking. In 2019, Insilico Medicine's GENTRL platform designed a novel DDR1 kinase inhibitor in just 46 days from target identification to synthesizable candidate, which was subsequently validated in animal models. [15] This kind of result was simply not possible before generative AI.

Table 1: Key AI Tools and Platforms Used in Drug Discovery

AI Tool /Platform	Category	Main Use in Drug Discovery	Key Strength
AlphaFold2	Deep Learning	Predicts 3D protein structures from amino acid sequence	Near-experimental accuracy; free access for all researchers
Chemistry42 (Insilico)	Generative AI	Designs new drug molecules from scratch	Generated novel drug candidate in 46 days
SwissADME	ADMET Prediction	Predicts how a drug is absorbed, distributed, and cleared	Free, fast, widely used in early screening
AutoDock Vina	Molecular Docking	Simulates how drug fits into target protein	Open source; reliable docking scores
DeepTox	Toxicity Prediction	Predicts toxicity of chemical compounds	Winner of Tox21 Data Challenge 2014
BenevolentAI Platform	Knowledge Graph + ML	Drug repurposing from biomedical data	Identified baricitinib for COVID-19 treatment
IBM Watson Health	NLP / Text Mining	Reads millions of research papers for drug-disease links	Identifies hidden patterns across massive literature
RDKit	Cheminformatics	Chemical structure analysis and molecular fingerprinting	Open source; widely used in QSAR modelling

AI IN DRUG REPURPOSING: FINDING NEW USES FOR OLD MEDICINES

Drug repurposing — also called drug repositioning — is the process of finding new therapeutic uses for medicines that already have regulatory approval or established safety data. The logic is simple: if a drug is already known to be safe in humans, the biggest hurdle in drug development (Phase I safety trials) can be greatly reduced or bypassed entirely. This means a repurposed drug can reach patients in 3–5 years rather than 12–15. [16]

AI has become the dominant approach to modern drug repurposing for a straightforward reason: repurposing depends on integrating multiple types of evidence simultaneously — gene expression profiles, protein interaction networks, drug mechanisms, clinical trial outcomes, patient records, and the biomedical literature. This is exactly the kind of large-scale, heterogeneous data integration that AI handles better than any other method. [17]

Network-Based Repurposing

Network medicine models the human body as a biological network — a map of thousands of proteins and genes connected by their interactions. Diseases occupy specific 'modules' within this network; drugs exert their effects by interacting with nodes nearby. AI systems can analyze the proximity between a drug's known targets and a disease module, predicting which existing drugs might have therapeutic activity against diseases they were never designed for. [18]

The COVID-19 Story: AI Repurposing in Action

The COVID-19 pandemic provided the most dramatic real-world demonstration of AI-powered drug repurposing. Within weeks of the SARS-CoV-2 genome being published, AI platforms around the world began scanning existing drug libraries against key viral targets — including the spike protein, the main protease, and RNA-dependent RNA polymerase (RdRp). [19]

BenevolentAI used its knowledge graph and machine learning platform to identify baricitinib — a drug approved for rheumatoid arthritis — as a potential COVID-19 treatment. The AI predicted that baricitinib would reduce viral entry into cells and dampen the cytokine storm response that kills many COVID-19 patients. This prediction was tested in the ACTT-2 clinical trial, where baricitinib combined with remdesivir significantly reduced recovery time in hospitalized patients. It has since received FDA Emergency Use Authorization and full approval for COVID-19 [20]

The entire journey from AI prediction to regulatory approval took less than two years — a process that would normally take well over a decade. This single case study changed how the pharmaceutical world views AI-powered repurposing.

REAL-WORLD CASE STUDIES: PROOF THAT AI WORKS

Theory and laboratory demonstrations are important — but what truly proves the value of a technology is whether it delivers results in the real world. The following case studies represent some of the most significant AI-driven achievements in drug discovery to date.

Insilico Medicine and Pulmonary Fibrosis

Insilico Medicine is a biotechnology company built entirely around AI-driven drug discovery. Using its integrated Pharma.AI platform, the company identified TNIK (TRAF2 and NCK-interacting kinase) as a novel therapeutic target in pulmonary fibrosis — a progressive and life-threatening lung disease with limited treatment options. The AI then generated and optimized a novel small molecule inhibitor, ISM001-055, which entered Phase II clinical trials in 2022. [21]

The total time from project initiation to clinical candidate selection was approximately 30 months — compared to an industry average of 6 to 10 years for the same stages. The cost was correspondingly lower. This case study is widely cited as one of the clearest demonstrations that end-to-end AI-driven drug discovery is not just theoretically possible, but practically achievable.

DeepMind AlphaFold2: Solving a 50-Year Problem

For decades, one of the hardest unsolved problems in biology was the protein folding problem — the challenge of predicting the three-dimensional structure of a protein from its amino acid sequence alone. This matters enormously for drug discovery because you cannot rationally design a drug to fit a protein if you do not know the protein's shape. Experimental determination of protein structures using X-ray crystallography or cryo-EM is accurate but slow and expensive.

In 2020, DeepMind's AlphaFold2 achieved a breakthrough that stunned the scientific community — predicting protein structures with accuracy comparable to experimental methods, for virtually any protein, in minutes. [22] The subsequent release of predicted structures for over 200 million proteins — covering essentially the entire known proteome of life on Earth — has given drug discovery researchers unprecedented structural data to work with. Targets that were previously considered 'undruggable' because their structures were unknown are now accessible.

BenevolentAI and Baricitinib for COVID-19

As described in the preceding section on the COVID-19 repurposing story, BenevolentAI's identification of baricitinib as a COVID-19 treatment represents one of the most consequential AI drug repurposing successes to date. [20] What makes this case particularly remarkable is the speed: the AI prediction was made in January 2020, clinical trials were underway by mid-2020, and regulatory approval was granted by 2021. The conventional alternative — starting from scratch to develop a new antiviral — would have taken years longer, at an enormous human cost.

MIT: Discovering a Novel Antibiotic with AI

In 2020, researchers at MIT published a landmark study in the journal Cell demonstrating that a deep learning model could identify entirely new classes of antibiotics. The model screened over 100 million molecular structures and identified a compound called Halicin — named after HAL 9000 from 2001: A Space Odyssey — that showed potent activity against drug-resistant bacteria, including Mycobacterium tuberculosis and Clostridioides difficile. Halicin had a molecular structure unlike any known antibiotic class, which would never have been prioritised by conventional screening. [9]

Indian Pharmaceutical Industry

India — the world's largest producer of generic medicines — is also actively integrating AI into its pharmaceutical research. Dr. Reddy's Laboratories has partnered with AI companies to accelerate lead optimization in oncology and metabolic diseases. Biocon has applied machine learning to protein structure analysis for its biosimilar programmes. Sun Pharma has explored AI-assisted clinical trial design to improve patient selection and reduce failure rates. Tata Consultancy

Services (TCS) has developed AI analytics platforms serving major pharmaceutical clients globally. [23] These developments position India well to move up the pharmaceutical value chain — from generic production to original AI-assisted drug innovation.

Table 2: Summary of Key Real-World AI Drug Discovery Case Studies

Organization	AI Technology Used	Disease / Target	Key Achievement	Time Saved
Insilico Medicine	Generative AI + Reinforcement Learning	Pulmonary Fibrosis (TNIK target)	Novel drug ISM001-055 reached Phase II trials	~30 months vs 10+ years
DeepMind	Deep Learning (AlphaFold2)	All human proteins (proteome)	Predicted structures of 200M+ proteins	Decades of work in months
BenevolentAI	Knowledge Graph ML	COVID-19 (JAK-STAT pathway)	Identified baricitinib; now FDA approved for COVID-19	2 years vs 10+ years
COVID Moonshot	AI-guided medicinal chemistry	SARS-CoV-2 main protease	Open-source protease inhibitor series developed	Months during active pandemic
Stokes et al. (MIT)	Deep Neural Network	Antibiotic resistance (E. coli)	Discovered Halicin — novel antibiotic class	Screened 100M compounds in days

ADVANTAGES AND LIMITATIONS: AN HONEST ASSESSMENT

Every transformative technology has both strengths and weaknesses, and AI in drug discovery is no exception. The following table presents a balanced, evidence-based summary of both sides.

Table 3: Advantages and Limitations of AI in Drug Discovery

✓ Advantages of AI in Drug Discovery	✗ Limitations and Challenges
Dramatically reduces drug discovery timeline from 10–15 years to 2–3 years	AI predictions are only as good as the data it learns from — garbage in, garbage out
Virtual screening evaluates billions of compounds digitally — faster and cheaper than lab testing	Many deep learning models are 'black boxes' — they give answers but cannot explain their reasoning
Early ADMET prediction eliminates toxic candidates before expensive clinical trials	High initial infrastructure cost — GPUs, HPC systems, and skilled data scientists are expensive
Generative AI designs entirely new molecules that human chemists may never have imagined	AI-proposed molecules are sometimes impossible to synthesise in a real laboratory
Drug repurposing via AI identifies new uses for approved drugs — saving safety trial time and cost	Regulatory frameworks for AI-designed drugs are still under development globally
AI integrates multi-omics data (genomics, proteomics) to find better biological targets	Risk of over-dependence on AI — clinical intuition and human judgment must not be replaced
Personalized medicine — AI designs treatments tailored to individual patient genetics	Algorithmic bias — if training data lacks diversity, AI predictions may not apply to all populations

The advantages listed above are not speculative — they are supported by the real-world case studies in Section 5. However, the limitations are equally real and must not be minimized. The pharmaceutical community's current challenge is not to decide whether to use AI, but to use it responsibly — building robust data pipelines, developing interpretable models, and working constructively with regulatory agencies to establish appropriate oversight frameworks. [24]

AI IN PHARMACY EDUCATION: PREPARING FOR THE FUTURE

The rapid adoption of AI in pharmaceutical research has direct implications for pharmacy education. A pharmacist or pharmaceutical scientist graduating today will work in an industry that is already AI-driven — and that will be far more so within a decade. Pharmacy curricula that do not include computational thinking, data literacy, and familiarity with AI tools risk producing graduates who are unprepared for the real working environment they will enter. [25]

Tools such as AutoDock Vina (molecular docking), RDKit (cheminformatics), SwissADME (ADMET prediction), and the AlphaFold Protein Structure Database are all freely available, well-documented, and suitable for incorporation into undergraduate pharmacy practicals. A student who can perform a molecular docking study, interpret ADMET predictions, and understand how generative AI works in drug design has a significantly stronger professional profile than one who cannot.

Leading international institutions have already recognized this. Harvard Medical School, MIT, and the University of Oxford have integrated AI-focused research programmes into their pharmacy and pharmaceutical sciences faculties. India's pharmacy institutions — including those affiliated with Jiwaji University — are well-positioned to follow suit, given the country's strong computational talent base and growing pharmaceutical industry. The combination of pharma domain knowledge and AI literacy is a rare and highly valuable skill set, both in India and globally.

FUTURE SCOPE: WHERE IS AI TAKING DRUG DISCOVERY?

The pace of progress in AI-driven drug discovery shows no sign of slowing. Several emerging developments deserve particular attention. Foundation models — large AI systems pre-trained on enormous biological datasets, analogous to GPT models in natural language processing — are beginning to appear for molecular biology. Models such as ESMFold (Meta AI) and ChemBERTa can be fine-tuned for specific drug discovery tasks with far less data than traditional models require, democratising access to powerful AI for smaller research groups and academic institutions. [26]

Multimodal AI — systems that can simultaneously process genomic sequences, protein structures, clinical records, and chemical structures — is moving from concept to practice. These systems

have the potential to integrate the full biological context of a disease into a single drug design workflow, enabling truly personalized medicine at scale. [27]

Quantum computing, while still in early stages, promises to dramatically accelerate molecular simulation — currently one of the most computationally demanding tasks in drug discovery. When combined with AI-driven molecular design, quantum-enhanced simulation could allow exploration of molecular space at a resolution currently impossible even with the most powerful GPU clusters. [28]

For India, the future is particularly promising. The country already has the world's largest pharmaceutical generic manufacturing base, a growing AI talent pool, and government initiatives such as the National Biopharma Mission that support pharmaceutical innovation. The convergence of these strengths positions India to become a major contributor to original AI-driven drug innovation — not just a manufacturer of medicines designed elsewhere.

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