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A Next-Generation Drug Discovery Using Artificial Intelligence: Achievements and Challenges - AI in Next-Generation Drug Discovery

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ABSTRACT

Artificial intelligence is revolutionizing drug discovery by accelerating target identification, molecular design, virtual screening, and toxicity prediction, while tackling longstanding challenges like high costs and lengthy timelines in traditional pipelines. This review explores recent AI innovations—such as AlphaFold for protein structure prediction, generative models for de novo drug design, and graph neural networks for drug repurposing—alongside real-world case studies from companies like Exscientia, Insilico Medicine, and BenevolentAI, which have produced clinical candidates like DSP-1181 and rentosertib.Despite these advances, key hurdles persist, including data quality issues, model interpretability, synthetic feasibility for complex molecules, and integration with experimental workflows, underscoring the need for explainable AI, better datasets, and ethical frameworks to bridge research gaps. Looking ahead, hybrid AI-experimental approaches and collaborations between pharma giants and AI startups promise to deliver safer, more personalized therapies faster.

Introduction:

Artificial intelligence (AI) is rapidly transforming the drug discovery industry by opening up previously unthinkable opportunities. From identifying promising drug targets to precisely forecasting molecular behavior, artificial intelligence has emerged as a powerful force behind faster and more accurate drug development. In recent years, AI-driven developments have begun to transform the traditional drug discovery process, providing pharmaceutical researchers with new levels of productivity, insight, and creativity. The field is still evolving at the same time, with growing interest in next-generation AI tools and recognition of important research gaps that need to be addressed.

However, the successful integration of AI depends on the quality of the data that is available, the ethical issues that are handled responsibly, and a realistic understanding of the limitations of computational models. This review unifies these themes—new advancements, present challenges, and future prospects—and looks at practical strategies like explainable AI, data augmentation, and integrating AI with conventional experimental techniques. The main objective of this article is to provide a comprehensive and objective analysis of how AI is transforming drug design and discovery, as well as what will be required to fully realize its revolutionary potential.[1]

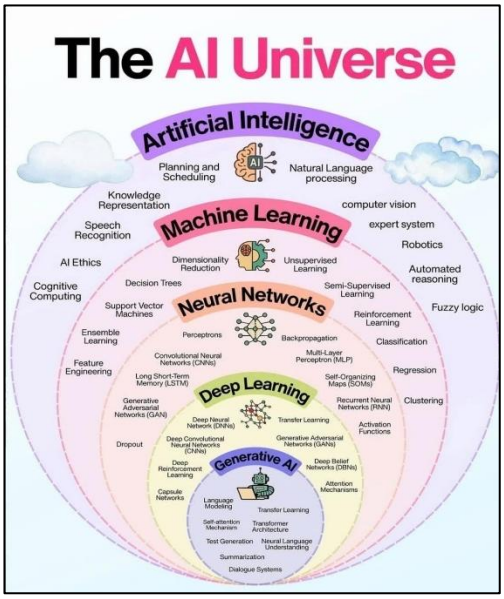

Figure 1: Illustration representing *"Overview of Artificial Intelligence and Its Subfields"*. Adapted from Blanco-Gonzalez et al. (2023).[1]

1. AI-Enhanced Drug Discovery Pipeline: Current Landscape and Emerging Applications

As shown in Fig. 2, a typical drug discovery pipeline consists of several crucial steps. Finding novel biological targets—typically proteins—that are connected to a specific disease is the first step in the target-based drug discovery process. Large chemical compound libraries are screened to find molecules that can interact with promising targets. The stability, activity, and general drug-like qualities of these initial hits are subsequently improved through refinement and optimization. Following optimization, the compounds go through preclinical research and several stages of clinical trials before moving on to regulatory approval if they show efficacy and safety. [2]

AI can now be used to improve nearly every stage of this pipeline. While reinforcement learning can fine-tune molecules to achieve particular desired properties, advanced generative models can create entirely new molecular structures. The use of graph-based neural networks to forecast drug-disease associations, find drug repurposing opportunities, and predict a patient's potential response to a specific treatment is growing. In addition to helping to automate certain steps in the regulatory approval process, natural language processing tools can extract insightful information from scientific literature.[3]

The creation of AI systems that can predict a protein's three-dimensional structure directly from its amino acid sequence—a crucial stage in structure-based drug design—has been one of the most revolutionary developments in recent years. By offering molecular structures, biochemical information, and molecular modeling tools, deep learning libraries and open scientific databases are now crucial in assisting this process.[4]

The atom becomes the fundamental unit for machine learning since drug discovery frequently concentrates on the three-dimensional structures of molecules, such as proteins, nucleic acids, and therapeutic compounds. AI can discover intricate patterns in these molecular systems through data. Graphs can be used to depict many relationships found in biomedical data, which makes graph-based machine learning particularly effective. This method can identify complex relationships between medications and illnesses, interactions between proteins, possible adverse effects, and even forecast how various patients may react to therapies. These models can highlight crucial molecular features like drug-binding sites or important interacting residues when paired with attention mechanisms, which improves the predictability and insight of the predictions.

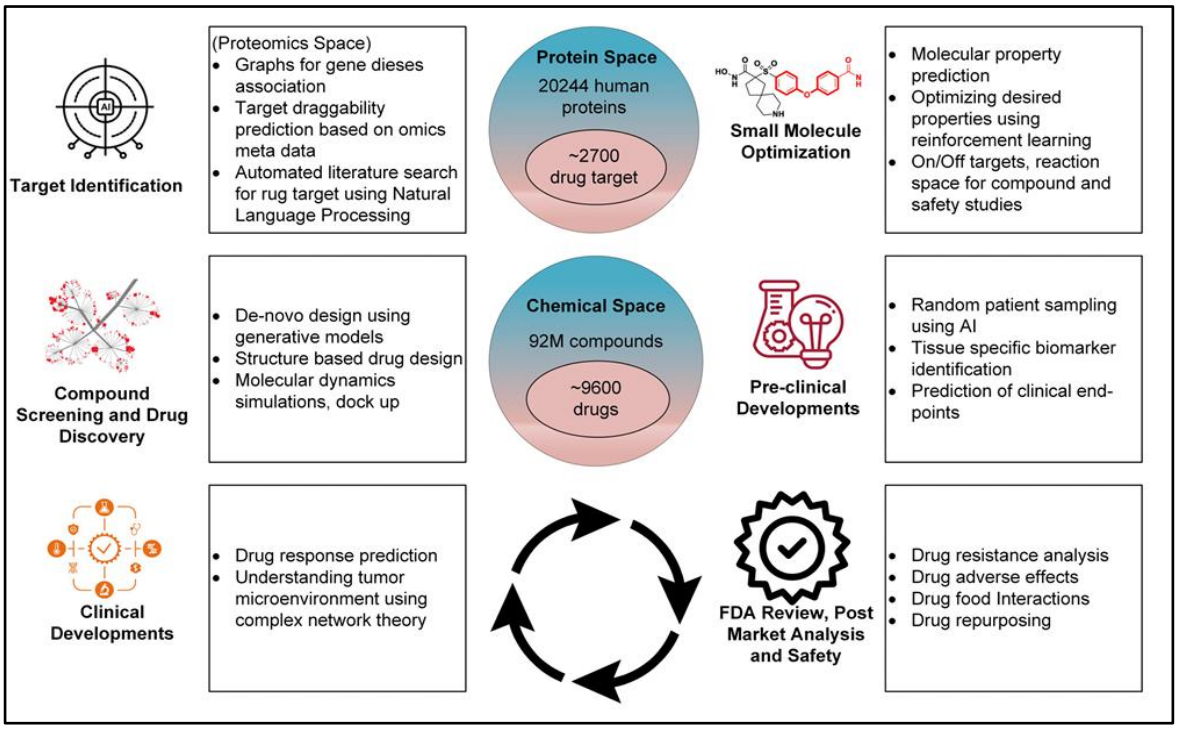

Figure 2: AI supports target identification, drug–target interaction prediction, molecular optimization, molecule generation, tumor microenvironment analysis, and literature mining for repurposing and regulatory insights.[5]

In the past, techniques like combinatorial chemistry and high-throughput screening were used to create new chemical entities. However, AI tools—particularly generative models, reinforcement learning, and graph neural networks—are becoming more and more able to design and optimize new molecules with a level of creativity and efficiency that can outperform manual methods. Later sections address these developments and how they are used in contemporary drug discovery.[5]

2. Application of Data Science in the Drug Discovery Process

The ongoing need for innovative treatments is highlighted by the ongoing emergence of infectious diseases and the rise in complex disorders worldwide. Target identification and validation, high-throughput screening, preclinical research, clinical trials, and regulatory approval are all common steps in the lengthy and resource-intensive process of traditional drug discovery. The pipeline's overall duration and cost demonstrate the need for more effective tactics.[6]

The development of artificial intelligence (AI) and data science has enabled powerful computational tools to aid in and speed up many elements of this process. These methods allow the discovery of novel therapeutic targets, a more comprehensive study of drug–target interactions, an increased understanding of disease mechanisms and faster lead optimization in small-molecule design. Besides, AI systems help to identify biomarker and predict drug efficacy, patient response, and resistance mechanisms.[7]

2.1 Target Identification in Drug Discovery

The goal of target identification is to identify biomolecules that play a role in disease progression when their activity is perturbed, typically proteins. Machine learning methods can use integrated data from various sources, such as gene expression profiles, protein–protein interaction networks, and wide-scale genomic and proteomic knowledge, to stratify candidate targets with therapeutic potential.[8]

While several thousands of proteins exist in the human proteome, only a small number are widely believed to be druggable today. Models constructed using AI could potentially enlarge this landscape by revealing novel links between genes, proteins, and disease pathways. Inference-based learning techniques and decision-tree algorithms can model causal relationships and network-level attributes relevant to the disease mechanisms.[9]

The academic literature continues to be one of the most important sources for target-disease relationships. The increasing use of natural language processing (NLP) tools to extract, classify, and curate relevant biological linkages enables the development of structured target-identification resources. Through similarity mapping of molecular features, a number of computational methods can predict drug-target interactions even in the absence of conclusive structural evidence.[10]

2.2 Virtual Screening and Optimization of Compounds

By forecasting the probability that a molecule will attach to a particular target, artificial intelligence (AI) plays a crucial role in virtual screening. These prediction models use information from known protein–ligand interactions, structural data, and molecular descriptors.[11] To inform molecule design, important physicochemical characteristics including solubility, ionization, permeability, and lipophilicity can be computationally assessed. AI-powered systems also facilitate early detection of unwanted chemical interactions, retrosynthetic planning, and the clarification of reaction mechanisms.[12]

Rapid investigation of vast chemical space is made possible by virtual libraries, which facilitate the effective removal of low-potential candidates. Multi-objective optimization frameworks can then be used to optimize molecules that have been identified as promising. The orientation, stability, and dynamic behavior of protein–drug complexes are further described via docking techniques and molecular dynamics simulations.[13]

2.3 Preclinical and Clinical Development

Making reliable predictions about the corresponding biological responses to the analyzed compound is an essential task preceding clinical trials. Machine learning models can be used to make binding affinity predictions, predictions about drug efficacy at the cellular level, or models of interaction patterns based on similarity or features.

In preclinical development, AI can assist with selecting patients through the mechanism of suitable biomarkers and highlighting possible toxicities or "off-target" effects. In clinical development, machine learning is being applied more and more to predict outcomes and risk assessment, leading to enhanced safety and fewer late-stage clinical failures. [14]

2.4 Regulatory Approval and Post-Market Analysis

Applications of AI range from drug development into regulatory and post-market domains. NLP-based systems can analyze scientific publications, clinical reports, and real-world evidence for the detection of adverse events, toxicity signals, and emerging resistance patterns. These will provide insights to support, at least partly, automate regulatory evaluations, patent documentation, and review workflows.

Off the back of approval, machine learning can predict market performance to help inform strategic decisions concerning manufacturing, resource allocation, and long-term management of the product. [16]

3. Key Technologies in AI-Driven Drug Discovery

Traditionally, the discovery of drugs was conducted through high throughput screening and empirical investigation, but currently, more modern approaches in artificial intelligence, mainly ML, DL, and NLP, allow for investigation and predictions in large biomedical data subsets. Each aspect mentioned above emphasizes the increasing role of artificial intelligence in developing drugs.[17]

AI models mimic basic cognitive capabilities, for instance, learning, perception, and language understanding; or decision support and data mining techniques. Though current technologies are limited to a niche AI application with a distinct task focus, they are important tools in molecular designing and decision support environments. Future research efforts seek to develop these technologies further while dealing with related challenges and concerns. [18]

3.1 A Fusion of QSAR, QSPR, and Structure-Based Modeling

This fact thus brings up the importance of drug design, which, over the last five decades, has combined AI with traditional modeling approaches like QSAR, QSPR, and structure-based methods. For a long time, QSPR and QSAR have formed the cornerstone for the prediction of biological activity and key pharmacokinetic properties. However, their capabilities have lately expanded manifold with the advent of modern machine-learning algorithms. Techniques such as support vector machines, gradient boosting, and deep learning models have nowadays enabled automated feature extraction and more accurate representation of complex molecular structures, including peptides and macrocycles.[19]

Research is ongoing to tackle issues like the availability of data and model interpretability, and strategies derived from natural phenomena and active learning. Simultaneously, structure-based modeling has been revolutionized by the adoption of deep learning models derived from computer vision to better predict protein-ligand interaction. Such developments reflect the successful merge of AI and classical computation for more accurate and efficient drug design.[20]

3.2 De Novo Drug Design with Artificial Intelligence

De novo drug design involves the design of new molecules with specific pharmacological attributes. The problem associated with the huge chemical space is the immense number of drug-like molecules contained in the space. The traditional ligand-based and structure-based designs are practical but hampered in their reliance on specific templates.[21]

This is a process that has been profoundly altered by the use of AI-generated models, which have been able to search the chemical space effectively in order to suggest the design of novel compounds thatare property-optimized. These AI models can be classified depending on whether they use a rule-based approach towards the design strategy or whether they apply a data-driven strategy that is rule-free. There are methods that can be used for the design of novel compounds.

Hybrid models combining rule-based and rule-free approaches are being viewed as potentially effective for the creation of bioactive and synthetically feasible molecules. Though at present most interest lies with ligand-based design approaches, interest for structure-based generative models for orphan targets or new molecules is growing exponentially. [22]

The discovery of AI methods has brought new hope to de novo drug design and A recent explosion in models, e.g, ReLEaSE[23], ChemVAE[21], Graph INVENT[24] and MolRNN[25] with a wide range of molecular representations have emerged.

3.3 Drug Toxicity Prediction

Prediction of drug toxicity is imperative in order to detect any toxic effect on patients and ensure patient safety. This was done through conventional approaches like laboratory experiments and animal studies, which are very expensive and have poor predictive values for human models.

Traditional methods are being replaced in this area using AI algorithms that leverage massive datasets of chemical properties, biological mechanisms, and known toxic values to build machine learning models. Such models identify intricate data patterns to predict toxic values quickly and correctly. [26]

Though AI enhances speed and predictivity, some hurdles are to be overcome, which include the requirement for quality data, interpreting models, and gaining acceptance in regulations. Nevertheless, AI toxicity predictivity possesses great latent potential to make drug discovery and development safer, more efficient, and more dependable. [26]

3.4 Integration of AI in Retrosynthesis and Reaction Prediction

AI tools have become important facilitators in the realm of retrosynthesis and reaction predictions and have brought a significant change in the process of designing a reaction route used in organic synthesis. With the application of machine learning algorithms to a collection of reaction data, predictions regarding forward and reverse reactions have become highly accurate and can be used to design reaction paths using graph search algorithms.[27]

AI-driven CAOS tools speed up the exploration of chemical space, help design novel molecules, and diminish tedious experimental trial-and-error. Though not without their challenges—like providing interpretability or adapting models to diverse chemistries—the ongoing collaboration between chemists and data scientists is rapidly moving these systems toward confidence and impact. [28]

4. Commonly Used AI Techniques

The choice of appropriate AI technology in drug discovery depends on the problem that is being solved. Almost all research work done in drug discovery falls into two broad categories based on machine learning models—supervised and unsupervised learning models.[28]

Supervised learning makes use of labeled examples for the training of the models, which are then capable of categorizing data or predicting the output for a given input. However, unsupervised learning deals with the use of unlabeled examples, where the patterns, groups, or structure are identified automatically. The techniques for supervised, unsupervised, and unsupervised learning of dimensionality reduction comprise classification, regression, clusters, and dimensionality reduction, respectively.[29]

In order to make these methods more convenient to implement, many open-source tools, including Scikit-learn, PyTorch, and Keras, have developed easily implementable algorithms. Some of the most popular approaches used in drug discovery using AI are enlisted in Table 1.[30]

Table 1. Widely used AI techniques in drug discovery[31]

Category	Task	Method	Representative application
Supervised learning	Regression analysis	MLR DT LR	DTI Adverse reactions Drug-drug interaction
	Classification	SVM CNN RNN GAN	Compound classification Bioactivity prediction *De novo* drug design Molecule discovery
Unsupervised learning	Clustering	*k*-means Hierarchical	Drug candidate selection Molecular scaffold analysis
	Dimension reduction	PCA t-SNE	QSAR Chemical space mapping

5. Artificial Intelligence In Drug Development: Present Status And Future Prospects.

There has been much advancement in the use of artificial intelligence in the discovery of disease pathways and the identification of novel targets. Using the combinatory power of genomics, biochemistry, and target suitability, artificial intelligence tools can effectively point out the target points better than the conventional approaches. There have been promising findings using platforms based on machine learning associated with the knowledge of gene to disease associations.

AI tools have also proved useful in unearthing novel mechanisms that were unknown. For instance, advanced AI systems have been instrumental in the discovery of novel RNA-binding proteins that interact with neurodegenerative conditions such as ALS. In a broad perspective, AI technology continues to transform early-stage drug development.[32]

5.1. AI in the Synthesis of Drug-Like Compounds

AI tools are being applied to assist with the synthesis of drug-like compounds that abide by Lipinski's rule of five. In retrosynthesis, the biggest issue is identifying the most appropriate reactions within a vast chemical space that are currently difficult to manually accomplish considering steric and electronic properties.

Despite this challenge, artificial intelligence retrosynthesis computer software predicts possible reactions and screens poor ones. More sophisticated computer software that incorporates neural networks and searching algorithms predicts possible synthesis routes faster and more accurately than conventional computer software. Yet, predicting stereochemical results and synthesis for extremely complex molecules remain problems that hang in the balance. [33]

5.2. AI in Identifying Hits and Leads

AI improves drug discovery, particularly in the early stages, as it is able to quickly screen chemical space and suggest new drug-like molecules. It is possible for machine learning algorithms to predict how a new drug interacts with a given target and at the same time optimize various properties related to safety and efficacy. AI helps filter and prioritize new molecules and ensures that as few as possible are made and tested for development.

In situations with scant information on structures, deep learning algorithms can resort to phenotypic, biological, or networking information to facilitate the identification of hits. Validated AI platforms increase the probability of success by choosing appropriate compounds and then categorizing them according to their feasibility of synthetic transformation from virtual to real constructs. [34]

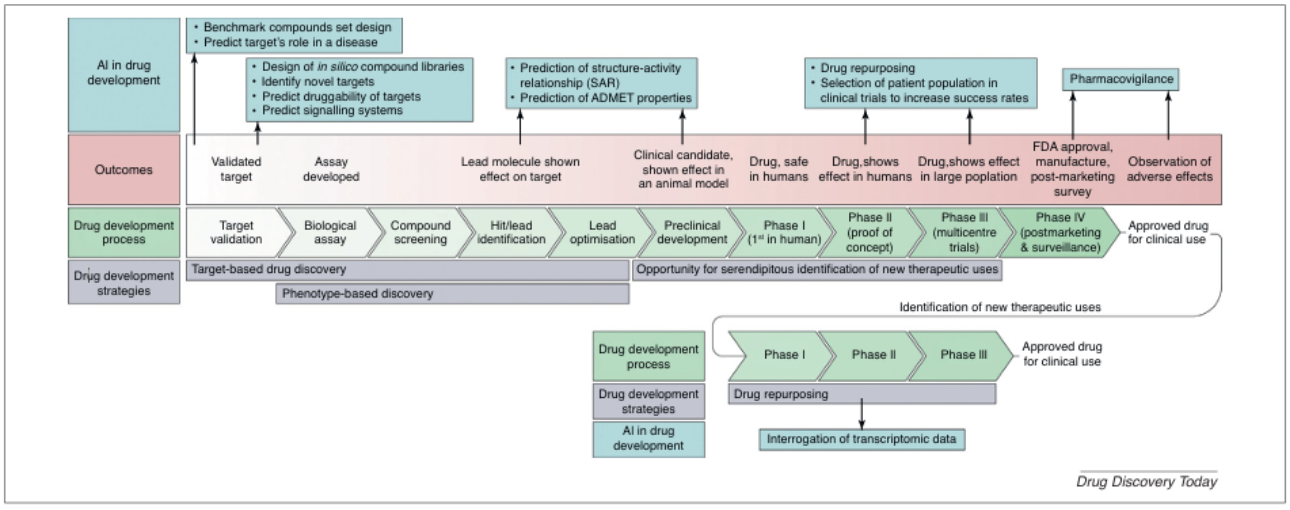

Figure 3: Use of AI for drug discovery. Results and design of the individual drug components are presented. The role of AI at each stage in drug development.[35]

5.3. AI in Drug Repurposing

AI has significantly enhanced the efficiency of drug repurposing by discovering fresh therapeutic applications of existing medications, a process which bypasses early-stage toxicity testing and proceeds directly to the later stages of clinical testing. Deep learning neural networks evaluate massive biological and transcriptomic datasets to deduce the mechanisms of medications, predict their class of therapy, and suggest fresh disease targets.

More complex architectures based on the neural network, generative adversarial networks, can even engineer novel molecules based on what they learned from actual biological molecules in the forms of chemicals, and the reinforcement learning setups explore designs in negligible reliance on labeled datasets. This can also be used to engineer safer medicines by identifying toxic molecules based on their gene expression modes and cardiotoxicity among different molecules.

New methodologies are catching up with the insight of medicinal chemists and are now attempting to limit human bias and optimize molecular discovery. On the whole, AI-powered repurposing facilitates faster and more informed discovery of potential therapeutic targets.[32]

6. AI and its applications in drug discovery

6.1. AI in Chemical Screening

The field of chemical screening has been revolutionized through the application of artificial intelligence. Machine learning algorithms such as Random Forests, Support Vector Machines, and Neural Nets can analyze large libraries of compounds at high-speeds to identify substances with desirable property profiles. The application of deep learning algorithms, especially those using convolutional neural nets, further improves this process. These algorithms analyze the intricate 3D molecular data to make predictions about their bioactivity with high accuracy. These applications make it faster to identify potential drug molecules.[36]

6.2 AI in Structure–Activity Relationship (SAR) Modelling

Another important application of AI is in structure-activity relationships, wherein it identifies the influence of minute variations in a molecule on its binding nature with biological molecules. Based on an analysis of vast amounts of data available for molecules, along with their activity profile, algorithms in this technology can even forecast the activity of new molecules. Thus, scientists can focus their initial efforts on molecules with highest priority, or promising molecules, resulting in an optimized drug discovery process. [37]

6.3 AI in Molecular Dynamics and Virtual Screening

AI is increasingly being used to assist in molecular dynamics simulation by predicting the behavior of molecules over time within biological systems. This is achieved through simulating the motion of atoms/molecules, which helps in testing the stability, interactions, and efficacy of a drug molecule prior to actual experimentation.

In the realm of virtual screening, AI analysis has enhanced ligand-based models in predicting bioactive compounds accurately. Various machine learning algorithms, including Naive Bayes, SVM, K-Nearest Neighbors, and decision tree models, show excellent performance in virtual screening based on optimized descriptors and fingerprints of molecules. Recent developments in graph neural networks have also shown improvements in the accuracy of predictions of various targets in cancer-related predictions and provided excellent results in both validation and test settings.[38]

7. Examples and Case Studies

7.1 AlphaFold (Google DeepMind)

AlphaFold, DeepMind's brainchild, represents a milestone in AI-driven drug discovery. With this system, the three-dimensional structure of a protein can be predicted with high accuracy directly from its amino acid sequence-a process that conventionally required several years of complicated laboratory research. With AlphaFold providing fast and highly accurate structural predictions, it significantly accelerates the identification of drug targets and supports the rational design of molecules able to interact with them. This has reimagined early drug discovery with reduced time, lower cost, and lower experimental uncertainty.[39]

7.2 DSP-1181: An AI-Designed Drug Candidate

DSP-1181 is seen as one of the first and most successful illustrations of an AI-driven approach for drug design. Developed by Exscientia in partnership with Sumitomo Dainippon Pharma, this drug, designed for use in patients with Obsessive-Compulsive Disorder, took about only a year to design, while typically this takes several years. A machine-learning approach has been used, whereby vast amounts of molecular data were scrutinized to optimize interactions with the target molecule, resulting in increased selectivity, efficiency, and success. In 2020, DSP-1181 marked an important achievement by becoming the first AI-discovered drug to begin trials in humans.[39]

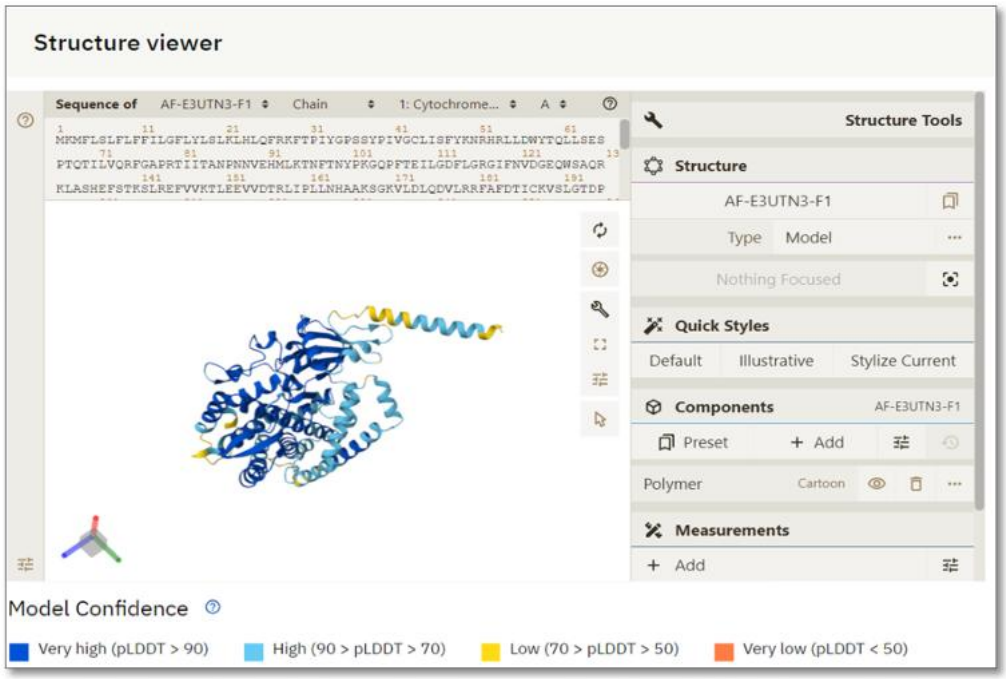

Figure 4: Screenshot of AlphaFold depicting the 3D structure of the protein CYP-450A (feeding input of a series of amino acids will result in the 3D structure prediction of the protein in space). Adapted from Saini, J.P.S., Thakur, A. & Yadav, D. (2025). RSC Pharmaceutics [39]

7.3 BenevolentAI and Drug Repurposing

One of the ways AI has impacted the development of medications is related to the use of AI in the repurposing of medications, including its use in the wake of the COVID-19 pandemic. A company called BenevolentAI, located in the UK, utilized sophisticated computer programming techniques in the form of algorithms. This was used on gigantic biomedical databases so as to determine which of the current medications could be utilized in the treatment of the virus. Some of the medications the company suggested included the use of baricitinib, a drug created to treat rheumatoid arthritis.[40]

Figure 5

Figure 6

Figure 5: ShareVault (2025) *Resources – BenevolentAI.* [50]

Figure 6: AI-enabled drug discovery collaboration between AstraZeneca and BenevolentAI. Source: Pharma Geek (2024).[51]

Exscientia and Personalized Medicine

Another significant example of innovation in the AI domain is that of Exscientia, which is associated with personalized oncology. The company uses AI to predict the response of patients to different therapies for the treatment of cancer, with the aid of personalized genetic and biomarker profiles. The technology enables the development of personalized treatment plans, which is essential in the field of medicine.[41]

Figure 7. Screenshot of AlphaFold that shows the 3D structure of a protein CYP-450A (feeding input as sequence of amino acids will output the 3D structure prediction of the protein in space). From Saini, J.P.S., Thakur, A. & Yadav, D. (2025). RSC Pharmaceutics

Exscientia unveils the first AI-designed immuno-oncology compound to enter clinical trials. Source: MedTech Alert (2023).[52]

Pfizer applied AI technologies throughout the development and manufacturing process of their COVID-19 vaccine to enable faster, smarter, and more dependable manufacturing processes. AI enabled them to predict possible disruptions within the supply chain, optimize the delivery of raw materials at the exact time they were needed, and also increase the manufacture while retaining the highest level of quality.[42]

Figure 8. Pfizer corporate building and logo. Source: Marketplace (2020).[53]

8. AI in Personalized Medicine and Pharmacovigilance

Artificial intelligence is revolutionizing patient care and the safety monitoring of drugs. With technologies such as machine learning and big-data analytics, artificial intelligence can enable physicians to provide treatment to patients that are specifically tailored to their requirements. It further enhances pharmacovigilance by spotting serious drug side effects at an earlier stage and facilitating real-time safety surveillance of drugs.[43]

8.1 Personalized Medicine

Personalized medicine tailors healthcare to each person, while AI makes it possible through analyses of genomics, among other biological data, guiding more precise treatment decisions.[44]

8.2 AI and Genomics

The AI system is able to handle huge amounts of genetic data in order to uncover the biomarkers that help predict the possible reactions of the human body to specific medicines. The machine learning algorithms, most importantly the deep learning algorithms, use the individual's genome, lifestyle, and medical history, in order to predict the most effective therapies, taking into account side effects.[39]

8.3 AI Platforms for Personalized Care

IBM Watson Health and Tempus are some of the tools that utilize advanced data analytic techniques that enable the identification of the most suitable options for a patient's treatment. And they integrate information from the genome, electronic medical records, and clinical research that enables more accurate decision-making. For instance, the tool, Tempus, uses AI technology that works alongside molecular information, allowing the oncologist to decide the most suitable cancer treatment that corresponds to the patient's unique genetic information.[45]

9. How AI Is Reshaping the Future of Pharmaceutical Innovation[46]

Drug discovery innovation is more important than ever because pharmaceutical spending is predicted to surpass US$1.9 trillion in 2027 due to the aging population and rising disease rates. In the typical multi-year process to bring the first drug to market, conventional drug discovery is too costly, time-consuming, and hit-or-miss.

AI is emerging today to eliminate the difficulties in this process. with the capacity to swiftly process vast amounts of data, forecast how new medications will behave, or alter clinical trials to speed up and improve efficiency. When DeepMind's AlphaFold model demonstrated extremely accurate protein structure predictions in 2018, the life sciences underwent a dramatic paradigm shift. This continued in 2020 when the COVID-19 pandemic prompted quick advancements in vaccines through AI-assisted scientific research, and in 2023 when highly targeted therapies were made possible by AI research incorporating multi-omics data.

Since then, Big Pharma has entered into more and more agreements with tech innovators. To advance AlphaFold-based technology, Eli Lilly and Novartis collaborated with London-based Isomorphic Labs. A young AI-biology startup called EvolutionaryScale recently raised a sizable sum of money and is collaborating with NVIDIA and Amazon Web Services to promote computational drug discovery. Simultaneously, Sanofi declared that it would expand its disease biology capabilities by implementing BenchSci's generative AI platform, Ascend, throughout its worldwide research facilities.

Together, these developments highlight how AI is ushering in a new era of smarter, faster, and more collaborative drug discovery.

10. Recent Milestones and Innovations in AI-Driven Drug Discover[47]

A major achievement has been realized by **Insilico Medicine** with the development of rentosertib, which is the first fully designed drug using generative AI. Its technology filters

promising drug candidates using end-to-end AI. Others have made significant progress. For example, AstraZeneca has shortened the time it takes to find new drugs thanks to a company called BenevolentAI, and Roche has adopted new techniques for biotechnological advancements that do not rely on animal testing. Here, they assess drug toxicity using organ-on-a-chip technology and artificial intelligence. India's Aurigene demonstrated how quickly the field is developing in 2024 by introducing an AI/ML-powered discovery system that reduces drug development time by roughly 35%.

Today's large language models, like ChatGPT, help researchers with a variety of tasks, from bioinformatics and literature reviews to statistical analysis and experiment planning. Chan Zuckerberg's rBio is another sophisticated tool that allows researchers to study digital models of cell behavior and pose complex biological questions in order to better understand how drugs might impact cellular functions. One recent innovation is the C2S-Scale 27B, a specialized foundation model created by Google in partnership with Yale University. This can lead to potential new treatments by providing a researcher with a "window into the cell" of potential targets associated with a specific type of cancer.

11. Prominent Companies Implementing AI in Drug Discovery & Development[48-49]

More and more big pharmaceutical companies are increasingly incorporating AI technology in their drug discovery processes. Big names in the drug manufacturing industry such as Pfizer, Genentech, Roche, Sanofi, Johnson & Johnson, and GNS Healthcare are using highly advanced AI technology in order to accelerate drug research, enhance precision, and reduce the expenses involved.

At the same time, a wave of innovative startups has emerged, offering cutting-edge AI platforms specifically designed to solve key challenges in drug design and development. Companies like **Exscientia, Roivant Sciences, Genome Biologics, BullFrog AI, DeepCure, Standigm, CytoReason, Insitro, Xtalpi, Absci, Postera, Atomwise, and Recursion** are becoming important players in this space.

Many have attracted significant investments and formed strategic partnerships with big pharma companies, further building confidence in using AI-driven ways to advance the development of new medicines.

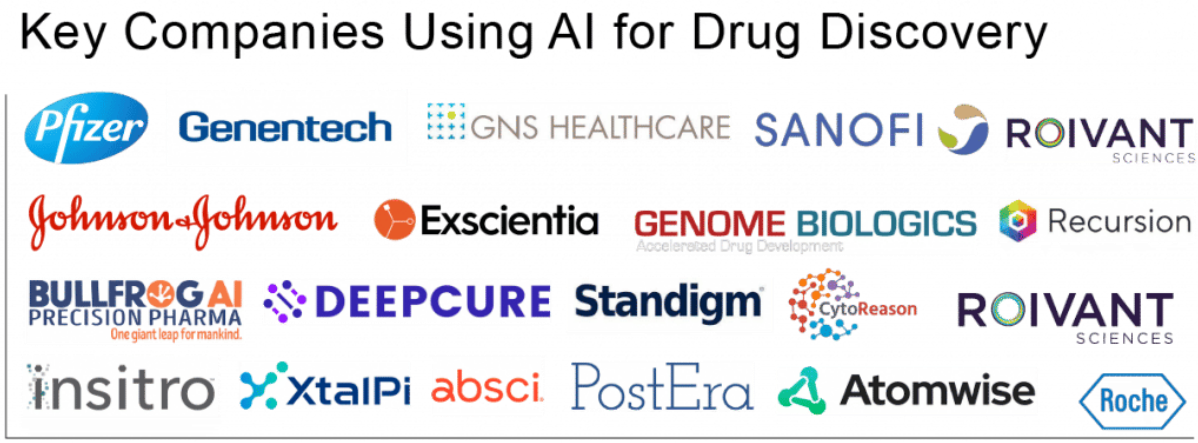

Figure 9. Key companies using AI for drug discovery. Source: DelveInsight Research (2022).[49]

RESEARCH GAP:

- **Data Quality and Availability:** Perhaps one of the most pressing challenges in developing an AI for use in identifying new medications is the availability of large, quality, and well-structured data sets. This is due to the fact that the data sets that have been available have been of low quality, inaccurate, and unstructured, thereby making it difficult for the AI to properly predict.
- **Models Interpretability and Explainability:** Presently, most of the models being developed by employing AI fall under the domain of so-called "black box" models. A simple example in this direction can be drawn from deep learning models, which, although giving results, do not describe the process they are employing to achieve the results. This in turn becomes a severe roadblock in approving such models, even questioning their authenticity.
- **Integration with Experimental and Clinical Workflows:** Although it is quite obvious that the AI techniques have great promise in the earlier stages like target identification or virtually screening compounds, the actual integration of the output resulting from the AI into the experimental or clinical workflows/processes is still in the developmental stage.
- **Feasibility of Artificial Synthesis and Complex Molecules:** Artificial synthesis feasibility, or chemical synthesis prediction using AI, faces a few challenges in terms of the prediction of complex molecules, specifically the prediction of stereo chemistry**.**
- Toxicity and Safety Prediction
- AI toxicity prediction tools for a drug have been improving, but more data and more interpretable predictive models would be necessary to easily spot potential safety issues in the early stages and avoid more instances of late-stage clinical failure.
- **Polypharmacology and Off-target Effects**: In order to maximize therapeutic benefit while

lowering the risk of unwanted side effects, current AI techniques need to be improved in order to better predict how drugs interact with multiple targets.

- **Drug Repurposing Validation**: Although AI has demonstrated encouraging results in proposing novel applications for currently available medications, translating these computer-generated predictions into approved therapies necessitates costly and time-consuming experimental validation and clinical trials.

- **Ethical, Regulatory, and Computational Limitations**: Using AI responsibly in drug discovery entails managing changing regulatory requirements, privacy concerns, and ethical issues. Additionally, ongoing research is necessary to meet pharmaceutical industry standards due to limitations in current computational resources and algorithm design.

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CONCLUSION:

The above are the main challenges yet to be harnessed to maximize AI's transformational impact in improving the drug discovery process.

Artificial intelligence is revolutionizing the drug discovery development landscape in ways never seen before, bringing about an unprecedented paradigm shift that is efficient, accurate, innovative, and revolutionary in terms of drug discovery development. The ability of artificial intelligence to analyze massive amounts of biological data and chemical data while at the same time being able to forecast interactions and compound builds has opened doors that were hitherto unimaginable.

Nevertheless, although these are impressive achievements, some tough challenges await us to be overcome to realize the full potential of AI. These are, in particular, issues related to data quality and availability, model interpretability, and integration in real-world experimental and clinical settings. In addition to that, better AI capabilities will be required for solving synthesis routes, safety prediction, as well as complex drug-target relations for the successful translation to a real-world scenario.

Ethical issues, regulations, and the accessibility of resources are some of the other variables which will contribute to the future of AI in the development of drugs. As the technology improves, inter-disciplinary collaborations are on the increase. I strongly believe that a new dawn is on the horizon where AI will not only expedite the development of drugs but also introduce a safe and effective remedy faster than ever before.

In the final analysis, in embracing the above challenges in the most innovative way, we will be able to unlock the true potential of AI in the pharmaceutical industry.

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