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Artificial Intelligence in Drug Discovery: Speeding up Innovation

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ABSTRACT

Drug discovery has traditionally been a prolonged, high-risk, and resource-intensive process characterized by low success rates and high attrition. The emergence of artificial intelligence (AI) has begun to transform this paradigm by offering scalable, data-driven solutions to longstanding challenges. This paper examines the multifaceted role of AI in expediting and enhancing the drug discovery pipeline, from target identification and lead optimization to de novo molecular design and drug repurposing. Key AI techniques, including machine learning, deep learning, and natural language processing, are discussed in the context of their application to various stages of drug development. Furthermore, the paper reviews case studies, data sources, and the integration of AI architectures such as generative models and graph neural networks. Despite its transformative potential, AI faces implementation challenges, including data sparsity, model interpretability, and ethical concerns surrounding privacy and bias. This review underscores how AI is not only speeding up innovation but also paving the way for more predictive, efficient, and cost-effective drug development strategies.

Keywords: Artificial Intelligence, Drug Discovery, Machine Learning, Deep Learning, Natural Language Processing, Molecular Modeling.

INTRODUCTION

Drug discovery involves identifying new medications for diseases through a multi-faceted process that includes basic research and utilizes various technologies. This process begins with identifying a biological target relevant to a disease, followed by the identification, synthesis, and statistical assessment of new drug candidates through biochemical assays and animal models. After the costly and time-consuming pre-clinical development, around 500 drug candidates may enter clinical trials, but typically only one is approved. The rise of high-throughput biotechnology has led to massive amounts of biomedical data, yet conventional discovery methods remain inefficient due to their low efficacy and high costs. To tackle this issue, there is a need for new methods to analyze large datasets in drug discovery. The advancement in high-performance computing and the availability of multi-omics data have allowed artificial intelligence (AI) techniques to move from theory to practical applications in areas such as social networks, cybersecurity, and transportation. There has been considerable interest from pharmaceutical companies in AI applications for biological data analysis, specifically in drug-target prediction and drug design. Major pharmaceutical firms are now collaborating with IT companies to create AI-driven drug design methodologies. A recent example includes Insilico Medicine's drug for idiopathic pulmonary fibrosis, which has shown positive results in initial clinical trials using a graph-based neural architecture. Thus, AI is revolutionizing drug discovery and development [1, 2].

The Role of Artificial Intelligence

The research and development of drugs to combat diseases is a lengthy and complex process. Artificial Intelligence (AI) has emerged as a potential solution to enhance drug discovery, significantly shortening timelines and improving research reliability. Many funds are globally invested in AI-driven drug discovery, prompting intense competition and numerous inquiries. This review outlines recent trends in

AI-guided drug discovery, covering areas such as target identification, hit identification, ADMET prediction, lead optimization, and drug repositioning. It summarizes key data sources and online resources while analyzing ongoing challenges and proposing future directions. New technologies intersecting molecular sciences, such as HTS, HTP, and various omics, are generating vast amounts of data and compounds, often leading to wasted efforts by researchers. Despite this, 80% of attrition reasons remain linked to poor pharmacokinetics, efficacy issues, and animal toxicity. Many small-molecule candidates have undergone ineffective target screenings, previously reliant on high-dose lipophilicity. AI-driven decision-making presents a breakthrough opportunity, offering innovative drug discovery approaches for both established and emerging diseases and optimizing chemical libraries while minimizing manual effort. Numerous groups are developing efficient AI-guided solutions for rational drug discovery, with recent architectures focusing on deep learning for molecular property prediction and compound optimization [3, 4].

Historical Context of Drug Discovery

In 1854, John Snow plotted the location of cholera cases and discovered a relationship between the disease outbreaks and water pumped from a specific source. The famous Broad Street water pump was removed. The drug discovery process must be able to learn enough knowledge from all accessible data. In general, a mobile phone increments both monologue and dialogue data continuously. The extra data can be exploited to learn more about fundamental properties of the phone, which can lead to a better model. Thus, the entire drug discovery process can be seen as a grand challenge about learning the mapping from drug to disease. In this sense, AI is an ideal candidate for discovering a generic drug discovery approach without worrying about the specific type of information or how well the data has been collected. Nevertheless, such a program has not been started yet 1. In most major companies with 'pharmaceutical' in their names, medicinal chemistry is a discipline. It is the physicochemical properties of drug candidates that determine bioavailability, specificity, safety, and drug-drug interaction. A good understanding of organ absorption and distribution mechanisms can help assemble and calibrate more phenotypes of synthetic compound libraries. These libraries, which should contain compounds with diverse structures, along with innovative sampling methods, make high-throughput screening easier. Drug repositioning is one of the hottest topics in the pharmaceutical industry. It consumes significantly less effort and resources compared with conventional drug discovery and development processes. With the proliferation of various biomedical resources, enormous opportunities have been generated for knowledge-based drug repositioning. Construction of new biomedical knowledge graphs, emergence of new reasoning approaches such as graph neural networks on structural tasks, and generative models on text generation tasks have a large potential to uncover new knowledge for repurposing existing drugs [5, 6].

AI Techniques in Drug Discovery

Drug discovery is a complex, challenging process requiring extensive knowledge of diseases, candidate medication design, and rigorous testing before market release. It begins with identifying disease targets, followed by target identification, molecular screening, lead optimization, and studies on pathology and toxicity. The investigational new drug application and clinical trials are necessary before a drug receives approval for general use. A typical cycle can take 10-15 years and cost billions, with only 1 in 5,000 candidates passing Phase 1 trials, making it a high-risk industry. AI has accelerated innovation, attracting over three billion dollars in investments in 2020, including the AI drug candidate DSP-1181 from Exscientia entering Phase I trials with Sumitomo Dainippon Pharma. Pfizer and BenevolentAI's collaboration yielded a preclinical candidate advancing to Phase 2 trials. However, drug de novo design presents complications; many virtual screening algorithms suffer from high false positive and negative rates. There is a pressing need for new techniques to overcome these issues. Advances in high-performance computing facilitate extensive computational chemistry on protein-ligand complexes, allowing for sophisticated statistical methods to analyze binding specificity. Furthermore, the proliferation of diverse chemical compound databases enhances query diversity, but challenges persist. The Hollywood Script Problem highlights difficulties in generating plausible drug-like molecules due to the combinatorial explosion of possibilities at the nano scale, which far exceeds the number of atoms in the universe [7, 8].

Machine Learning Algorithms

Advances in high-throughput screening, chemical synthesis, and genomics have accelerated new drug discovery; however, the actual time-to-market is typically many years. At present, with increasing enzymatic and chemical biology screening studies, the number of compounds becomes so large that it outpaces the native capabilities of most medicinal chemists and existing structure-based computer-aided drug design software. Rapid performance discovery is possible with existing HTE, but it is commercially

offered only at a limited number of service providers or in limited cases such as DNA-encoded libraries. Knowledge Graph, combined with QH-ML Cloud-AI, is expected to produce at least a first-pass model for protein-ligand discrimination, Z-score ranking, and hit discovery with a validation set, on a given target in 6 to 12 hours of steady-state computation. It is estimated that the work can be pushed forward to a level ready for physics-based simulation-refinement for one or more key candidates, within a few weeks for an original compound library of several million ligands. Practical applications to come off the workbench earlier with Compound Library Design 2.0, building upon Compound Library Design 1.0, Flatland 3D-Major League database for initial broad screening, and QH-ML-Ai-Compounds-for-Hit-Chemistry will be illustrated with some in-house examples. Machine Learning (ML), the subset of AI concerned with the design of algorithms that learn from data, has been successfully used to predict the properties of molecular compounds in the context of drug discovery. The success of ML in drug discovery has led to interest within industry and academia to develop and apply algorithms that solve predictive tasks in small-molecule drug discovery. Online machine learning works using data from an 'active' experiment, where molecules are designed and synthesized, to optimize performance in a 'passive' experiment, where the trained ML model suggests. Paradigms for both types of drug discovery use known compounds and assays to infer models that can be used to select the next experiment to perform. In practice, ML models can accelerate drug discovery, but they must be used iteratively with the experiment cycles [9, 10].

Deep Learning Applications

The utility of AI methodologies that have been applied to drug discovery, with a focus on deep learning. Understanding chemical and biological entities is an emerging area of research in AI. Based on molecular sequences, geometry, and bioactivity, deep learning has proven successful for molecular property prediction and drug design, which are the most popular applications of deep learning in drug discovery. Alternative structures are sought to overcome the shortcomings of small-molecule drugs, such as low selectivity and bioavailability. Protein-protein interactions are the majority of drug targets, but drugs are small molecules in most cases due to the challenges in accurate modeling of the protein-protein interface. The design of virtual screens to seek bioactive compounds to be drugs is booming due to the fast growth of compound libraries and their structural diversity. On the other hand, the ability to analyze high-throughput screening data is important for hit candidates to be drug leads. The broad application of different neural network architectures and newly developed methodologies, such as active learning, reinforcement learning, and molecular and protein design policies, are addressed. Trends of deep learning and AI in drug discovery are pointed and open challenges in need more effort will also be outlined. Most top publications are vulnerability discoveries in chemical understanding, molecular property prediction, generation of new metabolites, with efforts to characterize and visualize models, or designs of many data-efficient models, but with fewer industrial applications. Then, hundreds of applications on drug-related public datasets, and on test datasets that also show a significant speedup and accuracy improvement over previous methods addressing similar problems, are presented. Discrimination of active compounds from bioactive databases in multiple scale-up linked graphs, motifs, and tips are tested against a dozen GNN frameworks, privacy protection of fingerprints and descriptors by reconstruction or collage are also explored [11, 12].

Natural Language Processing

Deep learning has made significant strides in natural language processing (NLP), particularly in healthcare, finance, and mass media. This progress is driven by increased computational power and the availability of large-scale datasets, enhancing developments in computer vision and NLP. In drug discovery, where extensive text and structured data are available, NLP plays a crucial role in extracting insights that deepen scientific understanding. It focuses on learning models to interpret various text corpus types, including newspaper articles, clinical research abstracts, patents, and social media content. These data can be classified as structured, semi-structured, or unstructured. NLP applications in drug discovery are categorized based on supervised or unsupervised learning techniques, depending on pre-training. The initial step involves gathering a vast corpus of biomedical text, primarily from online media and scientific literature. While managing online media data follows standard NLP techniques, PubMed data requires specialized processing. Abstracts are retrieved via the Query API, though unrelated texts necessitate filtering algorithms, which may utilize keyword searches or trained classifiers. Text mining is an established field with refined processes for collecting and filtering data. Following filtering, preprocessing is often needed, including the removal of abbreviations, special characters, normalization, and lemmatization. Proper preprocessing enhances model training and improves performance. Tools and libraries for preprocessing can be leveraged, and current BioBERT and BioLM datasets allow for further

NLP model enhancement in drug discovery through ongoing pre-training with end-to-end pipelines [13, 14].

Data Sources for Drug Discovery

Drug discovery is a long process, typically taking 12-15 years, and about 90% of all new drug candidates that enter human clinical trials cannot be approved for marketing. Current methods for drug discovery are mainly based on chemogenomics resources and cheminformatics tools, which have made enormous contributions to current drug discovery. However, their low efficiency and high-cost characteristics have become hurdles to drug discovery. Therefore, the development of new methods to deal with such a time-consuming and expensive task is necessary. The recent revolution in high-performance computer hardware, coupled with the availability of multi-omics data, such as genomic sequence, gene expression, protein sequence, structure, and protein-protein interaction networks, has enabled AI/ML techniques to transcend from theoretical studies to real applications in multiple disciplines. The successful application of AI/ML techniques to biological data analysis has attracted the attention of pharmaceutical companies. Thus far, a variety of AI/ML techniques, including deep learning-based methods, have been implemented in drug discovery processes, such as drug-target prediction, bioavailability prediction, and de novo drug design. With the development of computer hardware and the increasing amount of biomedical data, drug discovery has gradually adapted to newer technologies. AI techniques include many machine learning algorithms, particularly deep learning algorithms, which have gained great success in various research fields, including drug discovery. By training machine learning algorithms with sufficient available data, the trained models can be used to predict unseen data efficiently. Consequently, the development and widespread use of AI techniques have opened up new opportunities for drug discovery since they can be used to analyze biological data. Some major pharmaceutical companies have begun to collaborate with IT companies to develop AI technique-based methods for drug design. Recently, the company successfully discovered a drug treating idiopathic pulmonary fibrosis with the help of AI, and the drug exhibits positive results in Phase I trials [15, 16].

Case Studies of AI in Drug Discovery

AI is revolutionizing drug discovery in many ways. The AI community explores innovative methods for this transformation. Most drug discovery milestones have been achieved using GPUs, with frameworks like BioNeMo and Biomed-LLMs enhancing data parallelism on BioGPUs. MegaMol, a geometric deep learning architecture, targets proteins at atomic resolution with over 15K molecular rigid-body pose degrees-of-freedom. It employs a specialized variational dynamic loss function for training with adaptive learning rates across the protein structure graph, ensuring model generalizability for unseen proteins. AI-GAN guarantees fidelity in generating drug-like structures, and MegaMol-GAN pre-trains a multi-modal architecture that produces protein-ligand structures for refinement in molecular dynamics simulations. In health research, resilient multi-modal architectures are explored, utilizing models in coevolution, protein languages, structural properties, and universal graphs, either generatively learned or engineered. A successful case of predicting novel biotherapeutic targets is noted using a 3D-Aware Graph Convolutional Neural Network (GCN). ActiveGraph is introduced to enrich biological knowledge, allowing for context-preserving subgraph queries in large-scale urban networks and reconstructing node embeddings, aiding the discovery of unseen nodes or edges [17, 18].

Challenges in Implementing AI

As the trend of using AI algorithms in drug discovery increases, limitations in data and current technology begin to surface. Concerns about data biases, ethical considerations, a lack of explainability, and patient privacy must be addressed before a comprehensive protocol for deploying AI in drug discovery can be established. The first challenge limiting the implementation of AI methods in drug discovery is the sparsity and bias of relevant data. Drug discovery datasets are notoriously sparse and biased, giving poorly informed results. Biased datasets can skew predictions towards low-quality or inaccurate results. Unfortunately, approaches to deal with data noise and biases in AI are not yet mature enough to be adapted for drug design and discovery. Additionally, while some datasets are publicly available, significant players in the field deliberately choose not to release their data, opting instead to "sell" the knowledge. This creates a scarcity of data on which academic research can be conducted. Neglecting the privacy preservation of drug discovery data can reveal sensitive information, leading to serious consequences. AI will likely require the integration of production-grade proprietary datasets or methods into its prediction models. This is a serious challenge for anyone looking to apply AI in drug discovery applications. While the idea of releasing black boxes that contain highly confidential private information is not a new concern in AI, it becomes significantly more intense in drug discovery applications. Current AI models deployed in different applications lack explainability, as it is generally

unclear how an AI-assisted drug discovery program has arrived at particular suggestions. While inaccurate predictions and suggestions can be improved, poor explainability makes identifying the possible reason behind the inaccuracies difficult. AI models must be integrated with models that can explain predictions on similar grounds as humans if they are ever to be considered trustworthy partners [19, 20].

Ethical Considerations

The rapid advancement of artificial intelligence (AI) in health and medicine presents significant ethical concerns alongside its opportunities. While AI holds promise for risk prediction, treatment personalization, and decision-making, it raises challenges related to safety, explainability, empowerment, privacy, fairness, accountability, and transparency. These issues have led to stricter regulations and calls for updated governance frameworks as public debate continues. This review analyzes 49 articles from the past 3 years on machine learning ethics in biomedicine, focusing on five key areas: safety, explainability, empowerment, privacy, fairness, accountability, transparency, governance and legislation, and education and trust. The goal is to identify gaps in understanding attitudes toward AI and outline future research directions. AI's transformative potential in pharmacology includes drug discovery, development, repurposing, and clinical trial design, but concerns about its regulation, validation, and application in pharmaceutical processes remain. Future discussions should address human expert involvement in AI tool design, access to AI models and datasets to combat the black-box issue, and the evolution of regulations that adapt to research advancements. Additionally, the potential for AI to generate biased datasets and questions regarding data provenance and its wider socio-economic and environmental implications warrant consideration. AI's impact may also extend to scientists not directly engaged in modeling, prompting the need for regulations akin to current biosafety standards to mitigate risks of fraud and safety violations [21, 22, 23].

Future Trends in AI And Drug Discovery

As AI and ML systems are increasingly established, uncertainty remains about their potential in drug discovery and future AI drug design steps. AI has successfully predicted the binding of small molecules to target proteins and desirable properties of candidate drugs, such as activity, toxicity, bioavailability, and solubility. A next step for AI might be to develop better metrics for evaluating model performance, especially in multimodal contexts. The field may benefit from generative modeling tools that can sample entire chemical spaces rather than sub-spaces. Sampling the vast chemical space presents foundational challenges in combinatorial design. Graph representations of small molecules are not unique, suggesting many drug-like molecules may meet model criteria. Data augmentation approaches could help models recognize equivalences in chemical representations, uncovering more drug-like options. Generative modeling based on cheminformatics, like fragment coupling and rule-based assembly, may accelerate hit generation. Chemical controllers to assess the validity and applicability of designs and predictions are essential. Questions on design validity and synthesizability can be addressed through rules-based approaches, but may introduce subjectivity. Additionally, drug discovery literature offers extensive knowledge on drug design rules and properties, which could enhance generative models' performance and provide insights into previously misunderstood design criteria [24, 25, 26].

CONCLUSION

Artificial intelligence is poised to fundamentally reshape the landscape of drug discovery by automating complex tasks, improving the accuracy of predictions, and significantly reducing the cost and time associated with drug development. From identifying novel drug targets to optimizing lead compounds and repositioning existing drugs, AI technologies offer unprecedented opportunities for innovation. Machine learning and deep learning models, supported by high-throughput screening, bioinformatics tools, and molecular simulations, are transforming how researchers approach problems that once took years to address. Nevertheless, challenges such as data quality, algorithm transparency, ethical considerations, and integration into regulatory frameworks must be resolved for AI to become a trusted and routine part of pharmaceutical research. Moving forward, cross-disciplinary collaborations between computational scientists, pharmacologists, and data engineers will be essential in harnessing the full potential of AI for healthcare breakthroughs.

REFERENCES

1. Nguyen MT, Nguyen T, Tran T. Learning to discover medicines. International Journal of Data Science and Analytics. 2023 Sep;16(3):301-16.
2. Chen W, Liu X, Zhang S, Chen S. Artificial intelligence for drug discovery: Resources, methods, and applications. Molecular therapy Nucleic acids. 2023 Mar 14;31:691-702.

3. Tiwari PC, Pal R, Chaudhary MJ, Nath R. Artificial intelligence revolutionizing drug development: Exploring opportunities and challenges. Drug Development Research. 2023 Dec;84(8):1652-63. researchgate.net
4. Blanco-Gonzalez A, Cabezon A, Seco-Gonzalez A, Conde-Torres D, Antelo-Riveiro P, Pineiro A, Garcia-Fandino R. The role of AI in drug discovery: challenges, opportunities, and strategies. Pharmaceuticals. 2023 Jun 18;16(6):891. mdpi.com
5. Mullowney MW, Duncan KR, Elsayed SS, Garg N, van der Hooft JJ, Martin NI, Meijer D, Terlouw BR, Biermann F, Blin K, Durairaj J. Artificial intelligence for natural product drug discovery. Nature Reviews Drug Discovery. 2023 Nov;22(11):895-916. knaw.nl
6. Nayarisseri A, Khandelwal R, Tanwar P, Madhavi M, Sharma D, Thakur G, Speck-Planche A, Singh SK. Artificial intelligence, big data and machine learning approaches in precision medicine & drug discovery. Current drug targets. 2021 Apr 1;22(6):631-55. researchgate.net
7. Vijayakumar H. The impact of AI-innovations and private AI-investment on US economic growth: An empirical analysis. Reviews of Contemporary Business Analytics. 2021;4(1):14-32.
8. Saad MF, Joudah NH. Financing and Investing in Artificial Intelligence: The Lucrative Benefits in Terms of Sustainable Digitalization. InInternational Conference on Explainable Artificial Intelligence in the Digital Sustainability 2024 Jun 19 (pp. 201-217). Cham: Springer Nature Switzerland. uobasrah.edu.iq
9. Ugwu CN, Ugwu OP, Alum EU, Eze VH, Basajja M, Ugwu JN, Ogenyi FC, Ejemot-Nwadiaro RI, Okon MB, Egba SI, Uti DE. Medical preparedness for bioterrorism and chemical warfare: A public health integration review. Medicine. 2025 May 2;104(18):e42289.
10. Aly M, Alotaibi AS. Molecular property prediction of modified gedunin using machine learning. Molecules. 2023 Jan 23;28(3):1125.
11. Wigh DS, Goodman JM, Lapkin AA. A review of molecular representation in the age of machine learning. Wiley Interdisciplinary Reviews: Computational Molecular Science. 2022 Sep;12(5):e1603. wiley.com
12. Martinelli DD. Generative machine learning for de novo drug discovery: A systematic review. Computers in Biology and Medicine. 2022 Jun 1;145:105403.
13. Wang M, Wang Z, Sun H, Wang J, Shen C, Weng G, Chai X, Li H, Cao D, Hou T. Deep learning approaches for de novo drug design: An overview. Current opinion in structural biology. 2022 Feb 1;72:135-44. [HTML]
14. Kim H, Kim E, Lee I, Bae B, Park M, Nam H. Artificial intelligence in drug discovery: a comprehensive review of data-driven and machine learning approaches. Biotechnology and Bioprocess Engineering. 2020 Dec;25:895-930.
15. Nguyen MT, Nguyen T, Tran T. Learning to discover medicines. International Journal of Data Science and Analytics. 2023 Sep;16(3):301-16.
16. Niazi SK. The coming of age of AI/ML in drug discovery, development, clinical testing, and manufacturing: the FDA perspectives. Drug Design, Development and Therapy. 2023 Dec 31:2691-725.
17. Vincent F, Nueda A, Lee J, Schenone M, Prunotto M, Mercola M. Phenotypic drug discovery: recent successes, lessons learned and new directions. Nature Reviews Drug Discovery. 2022 Dec;21(12):899-914. nih.gov
18. Pandey M, Fernandez M, Gentile F, Isayev O, Tropsha A, Stern AC, Cherkasov A. The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence. 2022 Mar;4(3):211-21. nature.com
19. Sadybekov AV, Katritch V. Computational approaches streamlining drug discovery. Nature. 2023 Apr 27;616(7958):673-85.
20. Gangwal A, Ansari A, Ahmad I, Azad AK, Sulaiman WM. Current strategies to address data scarcity in artificial intelligence-based drug discovery: A comprehensive review. Computers in Biology and Medicine. 2024 Sep 1;179:108734. [HTML]
21. Ugwu CN, Ugwu OP, Alum EU, Eze VH, Basajja M, Ugwu JN, Ogenyi FC, Ejemot-Nwadiaro RI, Okon MB, Egba SI, Uti DE. Sustainable development goals (SDGs) and resilient healthcare systems: Addressing medicine and public health challenges in conflict zones. Medicine. 2025 Feb 14;104(7):e41535.
22. Deng J, Yang Z, Ojima I, Samaras D, Wang F. Artificial intelligence in drug discovery: applications and techniques. Briefings in Bioinformatics. 2022 Jan;23(1):bbab430. [PDF]

23. Blanco-Gonzalez A, Cabezon A, Seco-Gonzalez A, Conde-Torres D, Antelo-Riveiro P, Pineiro A, Garcia-Fandino R. The role of AI in drug discovery: challenges, opportunities, and strategies. Pharmaceuticals. 2023 Jun 18;16(6):891.
24. Singh S, Kumar R, Payra S, Singh SK. Artificial intelligence and machine learning in pharmacological research: bridging the gap between data and drug discovery. Cureus. 2023 Aug 30;15(8).
25. Chatterjee A, Walters R, Shafi Z, Ahmed OS, Sebek M, Gysi D, Yu R, Eliassi-Rad T, Barabási AL, Menichetti G. Improving the generalizability of protein-ligand binding predictions with AI-Bind. Nature communications. 2023 Apr 8;14(1):1989. nature.com
26. Chatterjee A, Walters R, Shafi Z, Ahmed OS, Sebek M, Gysi D, Yu R, Eliassi-Rad T, Barabási AL, Menichetti G. Ai-bind: improving binding predictions for novel protein targets and ligands. arXiv preprint arXiv:2112.13168. 2021 Dec 25.

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