

Review Article

Artificial intelligence and computational tools in drug repurposing: a new frontier in therapeutic discovery

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ABSTRACT

Drug repurposing is the process of identifying novel therapeutic uses for currently available therapies that were initially created for different objectives in order to profit from the established safety and efficacy characteristics of well-known pharmaceuticals. Therefore, by avoiding the first phases of drug development, novel treatments can be introduced to the market more quickly and affordably. Artificial intelligence (AI) is a suitable substitute for conventional experimental approaches, which can be expensive and time-consuming, because of its lesser price, computer benefits, and capacity to reveal underlying trends. The primary subjects of this review include the use of AI algorithms in drug research and their unique and advantageous functions in identifying medicine repurposing, particularly when combined with in silico evaluation of therapeutic compounds. It has been shown that current AI systems are excellent at analyzing massive datasets, identifying intricate drug reaction patterns, and predicting potential medication repurposing. Building on these findings, there are still obstacles to establishing effective AI algorithms and carrying out further research, like expanding customized medicine, enhancing AI computing efficiency, and merging data-related databases for better repurposing.

Keywords: Computational drug discovery, Artificial intelligence, Drug repurposing, Precision medicine, Deep learning, Machine learning

INTRODUCTION

The process of discovering new therapeutic applications for drugs that are now available but were originally developed for different reasons is known as “drug repurposing”.¹ By using the documented safety and efficacy characteristics of existing drugs, this approach can significantly reduce the time, cost, and risk associated with traditional drug development.² This gives medical professionals additional therapeutic options and a workable way to meet unmet medical requirements. Clinically approved off-label, which reduces trial obstacles. The U.S Food and Drug Administration (FDA) has authorized a number of notable examples of successful drug repurposing, including the potential of

this approach as a viable means of addressing unmet medical needs.³ Trials can be carried out without the need for additional GMP production because drugs are already available. Due to its teratogenic consequences, thalidomide which were initially created and used to treat morning sickness in expectant mothers -was removed from the market. However, it was reintroduced into clinical practice after more research showed its effectiveness in treating multiple myeloma and leprosy.⁴ Another well-known example is sildenafil, which was sold as Viagra for the treatment of erectile dysfunction after initially being studied for cardiovascular disease. Repurposing, which is the process of discovering novel clinical applications, is another example of a drug. Uses for commercially available drugs that were first

developed for specific purposes, such as minoxidil, which was previously authorized as an antihypertensive. By utilizing the current safety and efficacy features of these medications, this strategy can drastically save the time, expense, and risk involved in traditional drug development. This is a useful tactic for addressing unmet medical practitioners. The medication was repurposed for the treatment of alopecia after clinical trials showed that it might stimulate hair growth. Computational technologies, ranging from network pharmacology and molecular docking to systems biology simulations and large-scale data mining, improve the prediction potential of AI-based methods.⁵ They work together to provide a holistic understanding of disease causes and therapeutic activities, facilitating hypothesis creation and rational candidate selection. This collaboration has accelerated reactions to new health risks (like pandemics) and enabled customized treatment approaches, opening up new avenues for therapeutic development. Medication repurposing possibilities are being redefined by the convergence of AI and computational approaches as the need for effective medication discovery grows. This new paradigm enhances the discovery process and paves the way for innovative, data-driven medical advancements. Additionally, minoxidil, which was first licensed as an antihypertensive medication, was changed to treat alopecia because clinical trials showed that it promoted hair growth. The following clinically proven cases highlight the enormous potential of drug repurposing as a strategy for reducing the risks involved with new medicine development while also providing patients with new treatment alternatives in a shorter amount of time. Drug repurposing is therefore a viable approach to both filling significant gaps in conventional medical care and finding potential therapies for illnesses for which there are now no effective treatments.⁶ AI-based modeling and computational techniques, which enable the rapid evaluation of large compound libraries and the identification of promising drug candidates without requiring significant laboratory work, can significantly reduce the time and money required during the early stages of drug development. The focus is on how AI uses target proteins and small chemical molecules to precisely and effectively find possible treatment candidates.

AI TOOLBOX FOR REPURPOSING DRUGS

Massive medical data resources

Drug repurposing is greatly aided by the vast medical databases that are accessible online all over the world.⁷ These databases are used to mine and analyze useful implications from these particular datasets, as well as to more verify the generated conclusions.

Pharmaceutical chemistry frequently offers the clearest indicator of a drug's efficacy in its intended use. Therefore, pharmaceutical chemistry's pertinent data resources aid in the discovery of more potent medications for a certain target. For instance, PubChem is an

extensive data repository for small molecules' biological activities that can provide details on the chemical structures, properties, biological activities, safety, and toxicity of many drugs. Statistical information on drug-like properties of bioactive compounds, particularly absorption, distribution, metabolism, and excretion (ADME), as well as target interactions and dangerous consequences.⁸ When examining pharmacological potential, the ChEMBL library's current mainstream machine learning models have proven to be quite helpful. Additionally, DrugBank is a database that incorporates all drug target data, such as pharmacokinetics, chemical structures, mechanism of action, and drug interactions. It has proven an essential tool for comprehending the molecular interactions and functions of drugs. The molecular mechanisms underlying these pharmaceutical wonders can be revealed by delving deeply into the complex world of drug activities using bioinformatics data, such as genomes, proteomics, and route information databases. Through omics study, reliable, data-driven genomic analysis can discover pharmacological targets and provide unmatched insights into drug molecular effects.⁹ Transcriptomics profile data can aid in navigating medication potential amidst expression patterns in the ever-changing realm of drug discovery, making it an effective tool for assessing and diving into the potentials of therapeutic interventions. The LINCS L1000 dataset, which comprises gene expression changes in human cells to diverse pharmacological perturbations on a genome scale, is a valuable tool for medication repurposing studies. Because L1000 records gene expression profiles for a wide range of medications, it is frequently used to discover novel clinical applications for previously licensed drugs. Different data formats have a clear impact on the interpretability of medication repurposing algorithms, exposing a variety of approaches for uncovering novel clinical applications for currently available pharmaceuticals.¹⁰ In addition to the previously mentioned DrugBank and LINCS, the Broad Institute provides the CLUE (connectivity Map) platform, which uses transcriptome data to compare disease gene expression profiles to drug-induced gene expression profiles in order to identify potential drug repurposing targets. Furthermore, analytical tools such as GNINA and deep chem can be hosted or integrated into web-based settings to perform tasks such as virtual screening, hence aiding drug repurposing research.¹¹

APPLICATIONS OF ARTIFICIAL INTELLIGENCE IN DRUG REPURPOSING

Repurposed drugs have been accelerated by artificial intelligence, which has turned the conventional trial and error method into a data driven, predictive, and economical procedure.¹² AI uses large biomedical datasets, sophisticated computational models, and pattern-recognition skills to more quickly and accurately find new therapeutic applications for currently available medications.

Repurpose drugs: a machine learning framework for identifying new therapeutic applications of existing medications

To overcome existing limitations and improve drug repurposing capabilities for researchers without programming skills, we present repurposed drugs, an ML-based web portal that offers a flexible approach to finding novel drug-disease relationships, including both single and combination therapies.¹⁷ From the clinical trials database, we carefully selected our dataset of drug-disease relationships. To increase the accuracy of the prediction model, a variety of descriptions were employed.¹⁸ Descriptors like ECFP4 (91024 bits) and ECFP6 (1024 bits), MACCS (166 bits), Klekota-Roth (4860 bits), Pubchem (881 bits), and Estate (79 bits) were used to encode the structural information in the 2D fingerprints.³³ 3D fingerprints (E3FP)³⁴ provided insights into spatial organization with a length of 4096 bits, while GNN-based fingerprints (3DInfoMax)³⁵ identified molecular graph topologies. It is important to remember that “context” refers to cross-validation out-of-fold predictions, which are generated by summing the predictions made on each validation set during the 10-fold-cross-validation. Even though the small dataset size results in a lower correlation for medication combinations, further developments with more trial data are anticipated to increase the model’s prediction module to focus on the most promising drug-disease connections by eliminating low confidence predictions using a default confidence threshold of 0.8. Furthermore, we have confirmed that Repurpose Drugs can forecast Phase I, Phase II, and Phase III. Repurpose Drugs’ anticipated approval likelihood for phase I compounds was 29%, which is indicative of this phase’s exploratory nature.¹⁹ In line with the emphasis on efficacy, Repurpose Drug’s anticipated approval likelihood rose to 38% for phase II trials. Specifically, Phase III studies demonstrated a significant improvement to a mean predicted chance of 63%, which is consistent with their advanced stage and near-market clearance. These findings show that our model can predict the chances of drug approval at different stages of clinical trials. Repurpose Drugs is expected to be a useful tool for the medication repurposing procedures and leveraging current data for forecasting.²⁰ It may greatly lower the expenses involved with conducting clinical studies and establishing clinical trial priorities by estimating the likelihood of pharmacological approval for specific applications ahead of time.

COMPUTATIONAL METHODS IN DRUG REPURPOSING

Computational drug repositioning has been proved to be a successful strategy for discovering new indications for currently available medications with lower risk and cost when compared to traditional drug discovery strategies.²¹ Target-based, gene expression-based, phenome-based, and multiomics-based approaches are only a few of the

numerous computational techniques that have been created. Many data sources are incorporated into the current upgrades, including biomedical databases and online health-related material.²² When anticipating new therapeutic indications, techniques that use target knowledge and drug structure have shown promise.

Structure-based computational methods

In drug research, molecular docking is frequently used to simulate drug-protein interactions. Molecular docking finds low-energy poses at drug-like chemical binding sites when conformations and ionisation states are generated.²³ Virtual screens are used to rate chemicals according to how well they connect to specific binding sites. A drug-like molecule is docked to several protein targets in inverse docking, a form of virtual screening, in order to select the most likely target.²⁴ Inverse docking experiments for target discovery have increased as a result of the COVID-19 pandemic.

Virtual screening and inverse docking software can combine a variety of techniques to increase robustness and reliability. These techniques frequently employ scoring functions, docking software, and ancillary tools such as pharmacophore models.

A number of docking programs, such as autoDock76, autoDock Vina77, and Glide78, offer unique features such as scoring systems and search techniques. The process of molecular docking involves a number of steps that affect the final docking results, such as tool selection, preparation of protein and molecule structures, investigation of potential binding sites, and normalization to eliminate compound size biases. For refining, molecular dynamics methods are commonly employed. Accurate estimates of binding free energy can be obtained by combining quantum mechanics scoring functions with machine learning (ML).²⁵ Optimizing medicine repurposing strategies and interpreting docking data can be aided by visualizing 3D structures and binding sites using programs like PyMol81 and chimera 80.

Ligand-based methods

Ligand-based methods are useful computational strategies for drug repurposing when the exact structural characteristics of the target protein are unknown. These methods leverage the chemical and biological features of known active components to forecast potential therapeutic applications for medications that are presently available. The essential premise is that identical pharmacophoric characteristics or structure are likely to result in comparable biological activities. Using molecular descriptors, physical features, and structural fingerprints, ligand-based approaches can quickly screen huge drug libraries and find candidates who may interact with disease-relevant targets.²⁶ Furthermore chemical similarity analysis using methods like molecular fingerprints and Tanimoto coefficients can reveal

structurally related medications with potentially comparable therapeutic effects.²⁷ All things considered, ligand-based methods offer insightful information on drug activity without the need for protein structural information. They are effective tools for speeding up drug repurposing and finding new therapeutic uses for already-existing compounds because of their capacity to forecast drug behavior based on chemical similarity, pharmacophore characteristics, and QSAR correlations.²⁸

AI MODELS FOR PREDICTING DRUG–TARGET INTERACTIONS

In recent times, artificial intelligence has become the transformational force in biomedical research, especially in drug discovery, which has traditionally faced substantial problems related to efficacy and efficiency.²⁹ The one drug-one target paradigm and high-throughput screening exemplify conventional drug delivery methods that often encounter challenges due to the intricacy of biological processes and the methodologies are costly, labor-intensive, and consistently result in considerable dropout rates during clinical trials, highlighting the pressing want for new alternatives. Artificial intelligence offers an effective answer to these difficulties by providing powerful algorithms that can analyze and understand intricate biological data with unmatched speed and precision. This ability to efficiently manage substantial data quantities has resulted in the creation of innovative techniques to comprehend complex biological mechanisms and the origins of diseases. This technological accomplishment signifies a paradigm shift in our approach to medicine creation, rather than a mere upgrade.³⁰ Simultaneously network pharmacology has gained prominence alongside AI in drug development. Network pharmacology provides an extensive framework for investigating the interconnections of genes, proteins, and metabolic pathways, emphasizing the complex linkages within biological networks. Algorithms of machine learning (ML) and deep learning can markedly reduce the time and expense linked to conventional drug development techniques by analyzing vast biological data to forecast prospective pharmaceutical prospects and their interactions with biological targets. However, by charting the intricate relationships between biological networks, network pharmacology provides a systems-level viewpoint that helps researchers find multitarget approaches and possible adverse consequences early in the development process.³¹

Target identification

Finding Drug Target Interactions (DTI) is crucial in the field of medicine and healthcare, where drug discovery is still a difficult task. DTIs show if a medicinal molecule has the ability to connect to target proteins and explain how these interactions take place.⁶⁴ Conventional techniques for detecting drug-drug interactions mostly depend on expensive and laborious in vitro and in vivo

studies.³² Moreover, there has been a notable advancement in this subject due to recent developments in computing approaches, especially artificial intelligence (AI) methodologies. AI techniques have several advantages, including quick prediction times, low costs, and high forecast accuracy.³³ AI-driven DTI prediction research has increased dramatically since the last ten years thanks to advances in processing power, increasingly complex AI algorithms, and the broad availability of data repositories including chemical, substance, and protein data. Although a number of review articles have been written about AI techniques for computational drug discovery, they frequently highlight particular strategies, such as deep learning, feature based, and molecular similarity-based machine learning strategies. However, a thorough overview of all AI methods in DTI prediction is still desperately needed.³⁴

NETWORK MEDICINE AND SYSTEMS-LEVEL COMPUTATIONAL TOOL

Network medicines is a new multidisciplinary area that uses system biology and network science to study illness and treatment methods at the system level rather than focusing on specific genes or targets. Computational methods at the system level, such as pathway analysis platforms, Protein-protein interaction network, gene regulatory network, platforms, and multiomics integration tools enable the building and study of these complex biological networks.³⁵ Using tools like Cytoscape, STRING, KEGG, Reactome, and Connectivity Map, researchers can discover similar pathways between diseases, discover disease modules, forecast drug target interactions and find possible drug repurposing prospects. Therefore, network medicine provides a thorough framework for understanding illness etiology, boosting precision medicine, optimizing multi-target therapy, and anticipating adverse drug reactions through data-driven, system-wide investigation of biological interconnections.

Disease–gene–drug network integration

In contemporary drug repurposing, techniques have developed into powerful instruments that enable the effective interpretation and analysis of enormous biological datasets. By exploring novel therapeutic indications for existing approved medications, drug repurposing time to save expense, and uncertainty that come with conventional drug development techniques. One of the most successful approaches in this area is disease-gene-drug network integration, which methodically integrates genetic variables, diseases, and the medications which are interacted with the targets in a huge quantity of biological and clinical data from a single computer model.³⁶ Disease–gene–drug network integration is based on the examination of transcriptomics, proteomics, genomes, and pharmacological investigations.³⁷ To identify links between genes and illnesses, OMIM, DisGeNET, and genome-wide association studies (GWAS) patient care,

Other databases that are used to identify gene-pharmaceutical interactions include DrugBank, ChEMBL, and the Comparative Toxicogenomics Database. They merge these various datasets and display them as linked networks, with nodes representing diseases, genes with nodes standing in for genes and illness and edges that stand for biological or pharmacological connections.³⁸ These interconnected networks offer comprehensive insights into therapeutic approaches and disease mechanisms. Illness, heredity, and medications combining computational and artificial intelligence techniques with disease-gene - drug network can lead to a major breakthrough in therapeutic discovery. This method accelerates the repurposing of pharmaceuticals, increases the probability of positive results, and promotes precision medicine using up to date biological data and advanced analytical techniques.³⁹ The potential for AI-driven network integration to transform drug discovery and improve despite ongoing persistent challenges including the need for experimental confirmation and the unpredictability of data.⁴⁰

DATABASES, PLATFORMS, AND COMPUTATIONAL RESOURCES

A number of databases offer crucial information to forecast DTIs, including information about ligand compounds, target proteins, and interactions. There are 17,085 compounds in the most recent version of Over 2.4 million bioactive drug-like compounds that have their 2D structures, various characteristics, and bioactivities stored in ChEMBL. More than 245 million protein sequences, functions, and characteristics are stored in UniProt. Moreover, fewer than 600,000 proteins have undergone expert evaluation and manual annotation.⁴¹ Over 82,000 proteins are thought to be present in the human proteome (UniProt Proteome: UP000005640). These experimental techniques are characterized by high costs and delayed development, yet they can yield extremely precise protein structural data. The field of protein structure discovery has completely changed by recent advancement of computational techniques, particularly artificial intelligence techniques, for protein structure predictions. Databases like BindingDB and PDBbind are used to categorize data regarding drug-target binding affinities.⁴²

Public datasets (DrugBank, ChEMBL, LINCS, etc.)

Beyond just offering a useful data source for research, ChEMBL's contributions to cheminformatics and drug discovery were crucial in accelerating method development in cheminformatics and related fields and encouraging more comprehensive approaches by providing a multi-target perspective on drug discovery. Additionally, over time, ChEMBL has sparked debate and established guidelines for FAIR and open data dissemination, making it a model for other open data providers. The latter has an impact on allied disciplines of study, such as bioinformatics subdomains that concentrate on the creation of biomedical ontologies.⁴³

Improving QSAR modeling has been one of ChEMBL's most important contributions to cheminformatics. Many researchers use ChEMBL as a source for creating predictive in silico models for particular protein targets or for a multitude of targets at once; the latter is frequently referred to as multi target QSAR because it provides organized and carefully selected data on chemicals and their biological activities. Methodological advancements in cheminformatics and related domains were also sparked by these discoveries.

The majority of compounds in the LINCS data set have several related gene expression patterns. In addition to repeat tests producing profiles under the same conditions, certain substances were screened at different concentrations and for different lengths of time, producing numerous profiles for a single agent. Each chemical has a different number of profiles; in MCF7 cells, the LINCS compounds linked to a DTXSID in RefChemDB had a median of six profiles. The individual may also provide a signature comprising a list of genes and proteins including those that are up- or down-regulated.⁴⁴

Transcript signatures for more than 15000 substances and genomic modifications of over 4,400 genes are examples of omics signatures. Transcriptomic and proteomic datasets are among the many illnesses covered by omics datasets that may be analyzed and used to create signatures.

AI-enabled repurposing platforms

AI-driven drug repurposing finds novel ways to treat uncommon illnesses using already-approved drugs. It uses the safety profiles of licensed medications to decrease risks and fill therapy gaps while cutting development time and expenses through quick data analysis. AI helps customized medicine, combines biological data to find drug-disease correlations, and encourages researcher cooperation. All things considered, this strategy improves the effectiveness and availability of treatments for uncommon illnesses.⁴⁵

AI-BASED METHODS FOR REPURPOSING DRUGS

Machine learning approach

Algorithms use large databases of drug-target interactions, side effects, and disease pathways to predict new drug-disease relationships. By combining pharmacological data and using better machine learning algorithms, AI innovation greatly improves medication creation. Deep learning approaches, which use both supervised and unsupervised methods for data clustering and prediction, are increasingly improving feature extraction and generalization.⁴⁶

Deep learning approach

Industry and research have a benefit from this machine learning technology that employs multi layered neural networks to retrieve data. Techniques like greedy layer-by-layer modeling help create complex models like DNNs, CNNs, RNNs, and autoencoders, especially in drug discovery. Pooling layers reduce spatial dimensions and calculations by operating independently on feature maps, which helps reduce overfitting and speeds up feature extraction. An AI method for processing and analyzing spoken or written data produced by humans is called natural language processing, or NLP. It analyzes text data using syntactic and semantic analysis.⁴⁷

Inference of network relationships from biological data, mainly from rapid experiments. Only a few researchers have used dynamic network modeling, while most have used static network modeling. Graph neural networks (GNNs) surpass deep learning models like CNNs. GNN models provide low-dimensional graph representations with nodal connection information.⁴⁸

Challenges and limitations

Validation and translational barriers

AI can be used in pharmaceutical product formulation at different phases of drug development, including possible target identification and validation, drug design and screening, drug repositioning, improving R&D efficacy, biological data analysis, quality control, pharmaceutical product management and patient selection for clinical trials. The search for novel therapeutics that will be successful in the future is expected to yield 1060 and 10100 viable compounds with potential interest in creating new medications possibly the most difficult aspect of the drug development process. A molecule is considered viable if it satisfies Lipinski's rule of five, a computational process used in drug discovery to predict a molecule's solubility, permeability, and pharmacological activity. The rule states that molecules must have a molecular weight of less than 500 Da, a LogP of less than 5, a number of hydrogen bond donors of fewer than 5, and a number of less than ten hydrogen bond acceptors. But the absence of advanced technology restricts the procedure of choosing feasible compounds and, as a result, the evolution of pharmaceuticals, creating this procedure expensive and time-consuming. AI might be used to address this issue.⁴⁹

Future directions

Multi-omics integration with AI

By enhancing productivity, accuracy, and speed at various phases of pharmaceutical research, AI is becoming more widely acknowledged as a transformational force in drug discovery. AI is crucial to the development of structure-based treatments, the

discovery of novel pharmaceutical targets, the repurposing of current substances, the prediction of toxicity, and the modeling of resistance mechanisms and pathogen-host dynamics.⁵⁰ Modern AI techniques, like machine learning, deep learning and natural language processing and generative models, facilitate the integration and analysis of massive multi-omics datasets, which comprise genomic, transcriptomic, proteomic, and metabolomic data. Important tasks including target discovery, pharmacokinetic prediction, de novo molecule design, and virtual screening are supported by these computational tools.⁵¹

Precision medicine and personalized repurposing

By combining machine learning and large data analytics using genetic research, the clinical implementation of precision medicine with artificial intelligence produces revolutionary outcomes in the search for drugs. In addition to being costly and time-consuming, the conventional approaches to drug discovery do not provide patients with individualized treatment. Fast genomic database analysis is now possible thanks to artificial intelligence, which helps produce personalized treatment for each patient. Researchers can predict how a disease will progress and determine the effectiveness of medications and their potential adverse effects by applying machine learning algorithms, which will improve the outcomes for patients undergoing genomic drug discovery.⁵² The analysis investigates the application of profound learning and reinforcement gaining knowledge about models for handling large amounts of genetic and biological data. Precision medicine can grow and become more effective thanks to high-performance computing systems and data storage via cloud computing platforms. By optimizing medication reuse analysis and encouraging new drug development procedures, AI computational biology in conjunction with clinical data improves pharmaceutical research. Through high efficiency, cost reduction, and the delivery of medication to specific patients, artificial intelligence is driving genomics-based drug discovery in a new direction. Despite persistent concerns such as data security issues, interpretation difficulties, and legal constraints, bioinformatics and artificial intelligence-based precision-based improvements advances personal medical care in the future.⁵³

Digital twins and predictive simulations

Digital twins (DTs) are a promising approach in this area. A DT uses real-time sensor data to continuously update its virtual depiction of an actual object, system, or even a human.⁵⁴ In the medical field, DTs function as virtual avatars by combining biometric, clinical and demographic information to generate comprehensive profiles of the patients.⁵⁵ DTs enable medical personnel to anticipate treatment outcomes and customize interventions by modeling and evaluating patient-specific situations. They

are becoming more and more recognized as a new area of customized medicine.⁵⁶

By conducting simulations in virtual environments, DTs are extensively utilized not just in the healthcare industry but also in the commercial and industrial areas to lower prices, reduce hazards and improve performance. Digital twins function within the Digital Twin Environment (DTE), independent of the stage at which the technology is being developed, tested or designed. Three primary categories of Digital Twins are identified in this analysis according to their implementation stage.⁵⁷ These include a digital twin prototype, or DTP, is created prior to the creation of a tangible product. In a virtual environment, it facilitates quick development and testing of predicted behaviours, materials, and design concepts.⁵⁸ Second the DTI or digital twin instance which is developed for an actual product that already exists. By creating a bidirectional, real time communication channel between the virtual and physical worlds, a DTI enables ongoing updates, validation, and monitoring.⁵⁹ Third is the digital twin aggregation (DTA): DTAs utilize cognitive skills to examine extensive amounts of data from physical items in order to monitor performance, adjust design and make interferences about how the product works and is used based on the facts.⁶⁰

CONCLUSION

Utilizing machine learning and algorithms using AI which has the ability to completely transform the process of finding new drugs and provide several advantages. The potential of AI to swiftly and effectively filter a large compound library is the most significant of them, as it significantly improves the identification of potential therapeutic candidates. Additionally, AI programs are able to offer invaluable perspectives and reduce the needs due to extensive preclinical and clinical studies by predicting the safety and effective characteristics of possible drugs. Artificial Intelligence's capacity for prediction has the capacity to increase the clinical trial success rate and speed up the process of developing of novel medications, resulting in the creation of safest and most potent medications. When applying AI to drug discovery, there are some problems that must be resolved. One of the main difficulties is the requirement for the collection of high-quality, diversified data. Furthermore, the interpretability of AI frameworks is essential for obtaining regulatory approval and building trust in the medical scientific communities.

In conclusion, the interaction between large data and AI in drug development is proof of humanity's never-ending quest for growth and knowledge. We are approaching a time where illnesses are more comprehensible, treatments are more tailored and every molecule that is studied, improved, and developed into a medication increases the chance of living a healthy life.

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REFERENCES

1. Kulkarni VS, Alagarsamy V, Solomon VR, Jose PA, Murugesan S. Drug repurposing: an effective tool in modern drug discovery. *Russ J Bioorg Chem*. 2023;49(2):157-66.
2. Ahmad A, Imran M, Sharma N. Precision nanotoxicology in drug development: current trends and challenges in safety and toxicity implications of customized multifunctional nanocarriers for drug-delivery applications. *Pharmaceutics*. 2022;14(11):2463.
3. Dhruva SS, Dusetzina SB, Phillips KA, Lynch HF. The Food and Drug Administration's role in supporting therapeutic development to address unmet needs: the National Academies report and beyond. *Health Aff Sch*. 2026;4(1):qxag013.
4. Bhatt P, Kloock C, Comenzo R. Relapsed/refractory multiple myeloma: a review of available therapies and clinical scenarios encountered in myeloma relapse. *Curr Oncol*. 2023;30(2):2322-47.
5. Suhani NS, Kumar S, Tiwari A, Upadhyay J, Nandave M, Ansari MN. Application of machine learning- and artificial intelligence-based tools in network pharmacology. In: *Network Pharmacology*. CRC Press; 2025: 55-66.
6. Weth FR, Hoggarth GB, Weth AF, Paterson E, White MP, Tan ST, et al. Unlocking hidden potential: advancements, approaches, and obstacles in repurposing drugs for cancer therapy. *Br J Cancer*. 2024;130(5):703-15.
7. Pan X, Lin X, Cao D, Zeng X, Yu PS, He L, et al. Deep learning for drug repurposing: methods, databases, and applications. *Wiley Interdiscip Rev Comput Mol Sci*. 2022;12(4):e1597.
8. Khare S, Chatterjee T, Gupta S, Ashish P. Bioavailability predictions, pharmacokinetics and drug-likeness of bioactive compounds from *Andrographis paniculata* using Swiss ADME. *MGM J Med Sci*. 2023;10(4):651-9.
9. Mukherjee A, Abraham S, Singh A, Balaji S, Mukunthan KS. From data to cure: a comprehensive exploration of multi-omics data analysis for targeted therapies. *Mol Biotechnol*. 2025;67(4):1269-89.
10. Cousins HC, Nayar G, Altman RB. Computational approaches to drug repurposing: methods, challenges, and opportunities. *Annu Rev Biomed Data Sci*. 2024;7(1):15-29.
11. Pan X, Lin X, Cao D, Zeng X, Yu PS, He L, et al. Deep learning for drug repurposing: methods, databases, and applications. *Wiley Interdiscip Rev Comput Mol Sci*. 2022;12(4):e1597.
12. Tiwari PC, Pal R, Chaudhary MJ, Nath R. Artificial intelligence revolutionizing drug development: exploring opportunities and challenges. *Drug Dev Res*. 2023;84(8):1652-63.

13. Naskar S, Sharma S, Kuotsu K, Halder S, Pal G, Saha S, et al. The biomedical applications of artificial intelligence: an overview of decades of research. *J Drug Target*. 2025;33(5):717-48.
14. Huang X, Li C, He Y, Liu B, Yan Q, Yu Z, et al. Repurposing GSK2018682 confers dual antibacterial and antibiofilm activity against *Staphylococcus aureus*. *ACS Infect Dis*. 2026;12(2):623-36.
15. Ochoa D, Hercules A, Carmona M, Suveges D, Baker J, Malangone C, et al. The next-generation Open Targets Platform: reimaged, redesigned, rebuilt. *Nucleic Acids Res*. 2023;51(D1):D1353-9.
16. Dara S, Dhamercherla S, Jadav SS, Babu CM, Ahsan MJ. Machine learning in drug discovery: a review. *Artif Intell Rev*. 2022;55(3):1947-99.
17. Meera M, Sekar S, Mahatao R. A novel approach for drug discovery-drug repurposing. *Natl J Physiol Pharm Pharmacol*. 2022;12(5):546-51.
18. Murali V, Muralidhar YP, Königs C, Nair M, Madhu S, Nedungadi P, et al. Predicting clinical trial outcomes using drug bioactivities through graph database integration and machine learning. *Chem Biol Drug Des*. 2022;100(2):169-84.
19. Akodad S, Niu X, Secades B, Stevens H. Impact of drug repurposing between 1985 and 2024 on pharmaceutical innovation. *Commun Med (Lond)*. 2026;6(1):84.
20. Bhatia T, Sharma S. Drug repurposing: insights into current advances and future applications. *Curr Med Chem*. 2025;32(3):468-510.
21. Li J, Zheng S, Chen B, Butte AJ, Swamidass SJ, Lu Z. A survey of current trends in computational drug repositioning. *Brief Bioinform*. 2016;17(1):2-12.
22. Sanches PH, de Melo NC, Porcari AM, de Carvalho LM. Integrating molecular perspectives: strategies for comprehensive multi-omics integrative data analysis and machine learning applications in transcriptomics, proteomics, and metabolomics. *Biology (Basel)*. 2024;13(11):848.
23. Pei Q, Gao K, Wu L, Zhu J, Xia Y, Xie S, et al. Fabind: fast and accurate protein-ligand binding. *Adv Neural Inf Process Syst*. 2023;36:55963-80.
24. Xu X, Huang M, Zou X. Docking-based inverse virtual screening: methods, applications, and challenges. *Biophys Rep*. 2018;4(1):1-6.
25. Adcock SA, McCammon JA. Molecular dynamics: survey of methods for simulating the activity of proteins. *Chem Rev*. 2006;106(5):1589.
26. Vázquez J, López M, Gibert E, Herrero E, Luque FJ. Merging ligand-based and structure-based methods in drug discovery: an overview of combined virtual screening approaches. *Molecules*. 2020;25(20):4723.
27. Bajusz D, Rácz A, Héberger K. Why is Tanimoto index an appropriate choice for fingerprint-based similarity calculations? *J Cheminform*. 2015;7(1):20.
28. Ahuja S, Kanwar D, Silakari P, Sahu SK, Kaur P. Medicinal chemistry perspectives on drug repurposing: innovative approaches and therapeutic breakthrough. *Ther Innov Regul Sci*. 2026;1-6.
29. Bassey GE, Daniel EA, Okesina KB, Odetayo AF. Transformative role of artificial intelligence in drug discovery and translational medicine: innovations, challenges, and future prospects. *Drug Des Devel Ther*. 2025:7493-502.
30. Chan SY, Loscalzo J. The emerging paradigm of network medicine in the study of human disease. *Circ Res*. 2012;111(3):359-74.
31. Abdelsayed M. AI-driven polypharmacology in small-molecule drug discovery. *Int J Mol Sci*. 2025;26(14):6996.
32. Lu Z, Song G, Zhu H, Lei C, Sun X, Wang K, et al. DTIAM: a unified framework for predicting drug-target interactions, binding affinities and drug mechanisms. *Nat Commun*. 2025;16(1):2548.
33. Zhu S, Yu T, Xu T, Chen H, Dustdar S, Gigan S, et al. Intelligent computing: the latest advances, challenges, and future. *Intelligent Computing*. 2023;2:0006.
34. Shi W, Yang H, Xie L, Yin XX, Zhang Y. A review of machine learning-based methods for predicting drug-target interactions. *Health Inf Sci Syst*. 2024;12(1):30.
35. Korcsmaros T, Schneider MV, Superti-Furga G. Next generation of network medicine: interdisciplinary signaling approaches. *Integr Biol (Camb)*. 2017;9(2):97-108.
36. Ma M, Huang M, He Y, Fang J, Li J, Li X, et al. Network medicine: a potential approach for virtual drug screening. *Pharmaceuticals (Basel)*. 2024;17(7):899.
37. Jiang W, Ye W, Tan X, Bao YJ. Network-based multi-omics integrative analysis methods in drug discovery: a systematic review. *BioData Min*. 2025;18(1):27.
38. Himmelstein DS, Baranzini SE. Heterogeneous network edge prediction: a data integration approach to prioritize disease-associated genes. *PLoS Comput Biol*. 2015;11(7):e1004259.
39. Wan Z, Sun X, Li Y, Chu T, Hao X, Cao Y, et al. Applications of artificial intelligence in drug repurposing. *Adv Sci (Weinh)*. 2025;12(14):2411325.
40. Ocana A, Pandiella A, Privat C, Bravo I, Luengo-Oroz M, Amir E, et al. Integrating artificial intelligence in drug discovery and early drug development: a transformative approach. *Biomark Res*. 2025;13(1):45.
41. Silverman EK, Schmidt HH, Anastasiadou E, Altucci L, Angelini M, Badimon L, et al. Molecular networks in network medicine: development and applications. *Wiley Interdisciplinary Reviews: Systems Biol Med*. 2020;12(6):e1489.
42. de Azevedo DQ, Campioni BM, Pedroz Lima FA, Medina-Franco JL, Castilho RO, Maltarollo VG. A critical assessment of bioactive compounds databases. *Future Med Chem*. 2024;16(10):1029-51.

43. Zhou Y, Hou Y, Shen J, Mehra R, Kallianpur A, Culver DA, et al. A network medicine approach to investigation and population-based validation of disease manifestations and drug repurposing for COVID-19. *PLoS Biol*. 2020;18(11):e3000970.
44. Pan Y, Lei X, Zhang Y. Association predictions of genomics, proteonomics, transcriptomics, microbiome, metabolomics, pathomics, radiomics, drug, symptoms, environment factor, and disease networks: a comprehensive approach. *Med Res Rev*. 2022;42(1):441-61.
45. Colak D, Nofal A, AlBakheet A, Nirmal M, Jeprel H, Eldali S, et al. Age-specific gene expression signatures for breast tumors and cross-species conserved potential cancer progression markers in young women. *PLoS One*. 2013;8(5):e63204.
46. Gangwal A, Lavecchia A. AI-driven drug discovery for rare diseases. *J Chem Inf Model*. 2025;65(5):2214-31.
47. Dara S, Dhamercherla S, Jadav SS, Babu CM, Ahsan MJ. Machine learning in drug discovery: a review. *Artif Intell Rev*. 2022;55(3):1947-99.
48. Fanni SC, Febi M, Aghakhanyan G, Neri E. Natural language processing. In: *Introduction to Artificial Intelligence*. Cham: Springer International Publishing; 2023: 87-99.
49. Farea A, Yli-Harja O, Emmert-Streib F. Understanding physics-informed neural networks: techniques, applications, trends, and challenges. *AI*. 2024;5(3):1534-57.
50. Ali KA, Mohin SK, Mondal P, Goswami S, Ghosh S, Choudhuri S. Influence of artificial intelligence in modern pharmaceutical formulation and drug development. *Future J Pharm Sci*. 2024;10(1):53.

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