Journal of Biosciences and Medicines, 2025, 13(5), 197-220
https://www.scirp.org/journal/jbm
ISSN Online: 2327-509X
ISSN Print: 2327-5081

AI-Driven Drug Repurposing for Oncology: Identifying Novel Cancer Treatments from Existing Drugs

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How to cite this paper: Ghimire, A. and Jain, P.T. (2025) AI-Driven Drug Repurposing for Oncology: Identifying Novel Cancer Treatments from Existing Drugs. *Journal of Biosciences and Medicines*, **13**, 197-220.
https://doi.org/10.4236/jbm.2025.135016

Received: April 9, 2025
Accepted: May 23, 2025
Published: May 26, 2025

Abstract

AI-driven drug repurposing is shaking things up in the world of oncology. It uses artificial intelligence (AI) to find new cancer treatments from drugs that are already approved by the FDA. This innovative approach taps into machine learning algorithms, extensive biological datasets, and sophisticated computational models to uncover potential new uses for medications that were initially created for different health issues. In oncology, where options can be limited due to challenges like drug resistance and the diversity of tumors, AI has the power to reveal fresh, effective treatment possibilities by sifting through complex molecular, genomic, and clinical data. This speedy identification of promising drug candidates can greatly cut down on the time, costs, and risks typically associated with traditional drug development. This paper dives into how AI is being applied in drug repurposing for cancer treatment, showcasing recent achievements, the merging of AI with clinical data, and the potential for tailored treatment strategies. It also looks at the hurdles in data integration, model validation, and getting regulatory approval, while pointing out future paths for the field.

Keywords

AI-Driven Drug Repurposing, Oncology, Machine Learning, Cancer Treatments, FDA-Approved Drugs, Drug Resistance, Tumor Heterogeneity, Personalized Medicine, Computational Models, Genomics, Clinical Data, Drug Discovery, Treatment Optimization, Molecular Analysis

1. Introduction

AI-assisted drug repurposing is changing the medical landscape, especially in cancer therapy, by opening new avenues for therapeutic interventions concealed within drugs already approved for clinical use in other pathologies. Whereas traditional methods can take years to characterize and extract drug-target interactions, now we can adopt modern approaches of deep learning to exploit the vast volumes of biological, genomic, and clinical data to find unforeseen interrelations between pre-existing medications and cancer-related molecular targets. The word "promising" seems appropriate in this case, more so since the treatment landscape is cluttered with the complexities attributable to tumor heterogeneity, genetic mutations, and patient-specific factors. A good case for this is the repurposing of metformin, a common medicine used for diabetes treatment that has shown some promise in inhibiting the growth of cancer cells in a number of tumor types. Similarly, thalidomide, often considered the drug against which all teratogens are compared, has now been successfully repositioned for treatment against multiple myeloma [1]. These examples accentuate the fact that AI can help bolster initial efforts in finding new indications for old medications, sometimes finding responsiveness, especially in cancers that resist conventional means of treatment.

Drug discovery, by any accounting, is extremely expensive and painfully slow, with new drugs taking over a decade and billions of dollars to gain regulatory approval. During this time, many promising compounds are still rejected at a late stage due to unforeseen safety or lack of efficacy. AI repurposing gives an immediate advantage by starting with drugs that already have undergone the sifting of safety and efficacy testing. This gives a high probability for clinical success and reduces the timeline from hypothesis to treatment extensively. Integrates genomics, proteomics, and real-world patient outcomes, gives precision that allows one to convert a one-size-fits-all model from a one-size-fits-all model to a personalized approach. It makes predictions regarding how a specific DNA type in a patient would be responsible for drug response informing selection of specific targeted therapies and drug combinations more likely to work. Findings from AI insights could spotlight neglected drugs and suggest hope to patients with rare or drug-resistant cancers, where normal investment from R&D is usually deficient. AI-enabled repurposing of drugs is not merely about speed or cost; it is about intelligence [2]. It opens up an entirely strategic, data-rich lens onto a process that has been historically rigid and expensive, enabling researchers to operate on significant patterns within vastly complex biomedical data. As this method matures, it will inevitably change the face of cancer treatment, delivering effective and personalized therapies at the same time as proliferating availability to patients around the world.

2. Methodology

AI-enabled drug repurposing fundamentally changes the oncology landscape in terms of discovering therapeutic applications for existing drugs. This involves the use of large biological, genomic, and pharmacological databases with already-approved compounds in the search for new possibilities of fighting cancer, rather than developing new compounds from scratch methodology that is time and cost prohibitive. Technology works best in terms of treating oncology because of challenges posed by tumor heterogeneity that make a treatment customized, as well as genetic variation and resistance mechanisms that modulate the response to standard treatment protocols. AI does not disrupt the enabling conditions by allowing the identification of hitherto unrecognized relationships between a molecular target and a drug that is already marketed. Such innovations allow faster and cheaper routes to new therapies. In this context, the success of AI applications is not only dependent on their powerful algorithms but also on the rigorous validation schemes delivered. As ontologies analyze networks of molecular structures, drug-disease interactions, and other types of multi-omics data, predictive accuracy must have been evaluated against established methodologies, particularly those based on statistics and computations. AI uses supervised machine learning techniques to measure performance in a pure traditional cross-validation, sometimes in k-fold and stratified bayes. Supervised machine learning models such as support vector machines and ensemble methods would typically be validated through cross-validation techniques, often k-fold or stratified variants, to ensure the generalizability of their findings. Such validations help confirm that a model trained on one subset of the data can reliably predict outcomes on unseen cases, a key requirement for translating insights into clinical trials. Performance B OMSometimes tested individually or by orthogonal data sets, such as pharmacogenomic databases like GDSC or CCLE, on performance with the old test set or an independent external validation, relative to the former between the two. Performance is measured by metrics with clinical relevance: sensitivity (true positive rate), specificity (true negative rate), precision (positive predictive value), and area under the curve of the receiver operating characteristic (AUC-ROC). It measures profit withdrawal from data, just as privacy leads to a better understanding of meaningful differences between drug-disease relationships that have been identified and falsely attributed. Particularly in oncology, such "false positive" leads can result in expensive and damaging clinical errors. New Classification Class I and II Use multi-class and regression-based models validated by the metrics given below: adjusted R^2, mean squared error, and concordance indexes depending on what endpoint is modeled-drug response levels, tumor shrinkage percentages, and predictions of survival time. Most models are high-dimensional, integrating multiple data types, such as genomic profiles, transcriptomics, and actual clinical records, but are stratified by cancer subtype or mutation status for the performance metrics, so that predictions. In this way, they could be expected to hold well across different types of biological backgrounds. This becomes most relevant in precision oncology, where treatment may differ significantly depending on a patient's actual molecular signature.

In contemporary science, the importance of interpretability and reproducibility in model evaluation is increasing. The explainable AI techniques such as SHAP (SHapley Additive exPlanations) and LIME (Local Interpretable Model-agnostic

Explanations) are being used more frequently to validate the correctness of a model and the reasons behind its predictions. Thus, the approach provides significant accountability requirements for regulatory approval and clinical acceptance, actuating clinicians to trust and acting upon the recommendations of the model. These rigorous validation strategies confer scientific credibility and clinical actionability upon the AI-driven approach to drug repurposing. When designed and deployed properly, these models are covered with highly validated evidence the high predictability that the repurposed drugs will have when entering a clinical trial. Validation protocols further turbocharge the AI-envisioned speed, cost-cutting, and precision in elevating the prospects for AI to make a transformational impact in oncology. By embedding validation of models deeply into every stage of AI-supported discovery, the field ensures that this powerful technology generates not mere hypotheses but clinically pertinent, reproducible, and high-confidence insights. Speedy, precise, and trustworthy: this is what transforms AI drug repurposing from a novel concept into a necessity in the war against cancer.

3. Overview of Drug Repurposing

Drug repurposing, often referred to as drug repositioning, is all about finding new therapeutic uses for drugs that have already been tested and approved for other medical conditions. This approach takes advantage of the established safety profiles of these medications, aiming to broaden their therapeutic potential to tackle different diseases. The core idea behind drug repurposing is that drugs, which were initially designed to target specific pathways or conditions, might actually have wider applications that weren't recognized at first. By exploring these additional uses, researchers can sidestep many of the early hurdles faced in traditional drug discovery, like proving safety and understanding basic pharmacological properties. This makes drug repurposing a more efficient alternative to the long and expensive journey of creating entirely new drugs from the ground up. In the healthcare landscape, drug repurposing is crucial as it addresses unmet medical needs and accelerates the process of getting new treatments to patients [3]. This strategy is especially important for diseases that are tough to treat or where current options are limited. Take oncology, for instance—cancer therapies often grapple with issues like drug resistance, treatment effectiveness, and how individual patients respond. By repurposing existing drugs, many of which have already undergone thorough testing, we can tackle these challenges more effectively, providing quicker and potentially safer alternatives. Plus, drug repurposing can lead to the discovery of treatments for rare or complex cancers that would otherwise take years to develop using traditional methods.

In the world of oncology, drug repurposing brings a treasure trove of advantages. The most striking benefit is its cost-effectiveness. Creating a new cancer drug can be a staggering financial burden, often racking up millions of dollars and taking years of research and trials. In contrast, repurposed drugs have already navigated many regulatory hurdles, which significantly cut down on the time and costs tied to preclinical and early-stage clinical development. In fact, the expenses associated with clinical trials for these repurposed medications are usually much lower since they've already proven safe for human use. This quicker development timeline not only means faster access to new cancer treatments but also allows for the introduction of therapies when they're most needed, particularly for aggressive cancers that demand swift action. The historical success of drug repurposing shines brightly in cancer treatment. A prime example is chloroquine, an anti-malarial drug that was discovered to have potential anti-cancer effects. Originally used to combat malaria, chloroquine was repurposed because it can inhibit autophagy, a process that some cancer cells depend on to survive. Clinical trials are currently underway to evaluate its effectiveness when combined with other cancer therapies [4]. Another well-known case is doxycycline, an antibiotic that has shown promise in clinical studies for its ability to hinder cancer cell metastasis. These examples highlight how repurposing existing drugs not only paves the way for new cancer treatments but also enhances treatment strategies by targeting specific mechanisms related to different cancers. In addition to the examples mentioned, there are quite a few other medications that were initially created for different illnesses but have now found new life in cancer treatment. This really highlights the incredible potential that drug repurposing holds in the field of oncology. Thanks to cutting-edge technologies like artificial intelligence (AI), researchers are getting better at spotting and predicting new uses for existing drugs, which is opening up some thrilling new avenues for cancer care. As AI algorithms dive into complex biological data—like genetic information and the unique traits of tumors—they're offering us amazing insights into how and why certain drugs can be effective against different types of cancer. Drug repurposing is a smart and incredibly valuable strategy in healthcare. It brings a host of benefits, including reduced costs, quicker development times, and better access to treatments. This approach is especially important in oncology, as it opens up exciting new avenues for finding innovative cancer therapies. The successful historical cases of drug repurposing really showcase its potential and underline how it can transform cancer treatment, giving new hope to patients who are looking for effective and accessible options.

4. Role of Artificial Intelligence in Drug Repurposing

Artificial intelligence (AI) and machine learning (ML) are becoming essential players in the world of drug repurposing, particularly in oncology. What makes this shift so significant is AI's remarkable ability to sift through enormous amounts of complex biological, molecular, and clinical data that would be overwhelming for human researchers to handle. Traditionally, finding new uses for existing drugs has been a slow and tedious process, often involving painstaking manual analysis and a lot of trial and error. But with its powerful computational skills [5], AI speeds things up by quickly spotting patterns, connections, and potential treatment opportunities that might slip through the cracks in standard research methods.

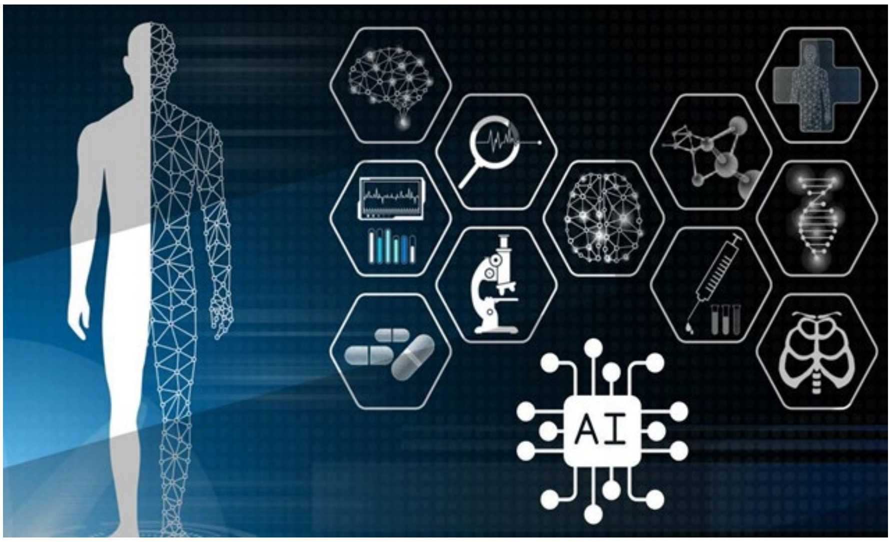

Figure 1. This image shows the role of AI in drug repurposing.

Figure 1 portrays how artificial intelligence and machine learning are incorporated into health care and medical research. Shown left is the figure of a human being transformed into a digitalized mesh, which indicates the digitization of human biology. Connected hexagons shown right represent different AI applications in medicine such as diagnosis, drug discovery, genomics, imaging, data analysis, personal treatments, and molecular biology. The central AI icon, on the other hand, indicates that AI is the fundamental enabler, powering insights and decisions across these domains by analyzing vast datasets, recognizing patterns, and accelerating innovation. In total, the design indicates that modern medicine is progressing towards data orientation and precision, thanks to the impact of AI.

AI systems excel at analyzing large, multidimensional datasets that are crucial for drug repurposing. These datasets encompass genomic information, which reveals the genetic structure of tumors, along with proteomic and transcriptomic data that shed light on protein expressions and molecular pathways. Clinical data, including patient records and treatment responses, are also woven into AI models, enabling researchers to fine-tune their predictions based on real-world results. By processing this diverse array of data, AI can uncover hidden links between drugs and cancer-related targets. For instance, by examining how different drugs interact with specific genes or mutations tied to cancer, AI can suggest whether a drug, originally designed for a completely different illness, might also be effective against cancer cells. One of the standout features of AI in drug repurposing is its knack for predicting how existing medications interact with specific cancer-related molecular targets. By training AI models to recognize the molecular structures of these drugs and how they interact with cancer pathways, we can gain valuable insights. When this information is compared to a vast database of known drug mechanisms and genetic mutations associated with cancer, AI can recommend which drugs might work well against particular tumor types, even if those drugs weren't initially intended for that use. This ability to predict outcomes means researchers can pinpoint promising drug candidates much more quickly than with traditional methods, allowing them to concentrate on the most promising repurposing opportunities [6].

A variety of AI techniques play a role in this process, with deep learning, natural language processing (NLP), and predictive modeling being among the most crucial. Deep learning, which is a branch of machine learning that emulates how our brains process information, excels at spotting patterns in large datasets. In the realm of drug repurposing, deep learning algorithms can sift through molecular and clinical data to uncover correlations that might suggest a drug's potential effectiveness in treating cancer. These neural networks, made up of layers of interconnected nodes, analyze data in multiple stages, enhancing their accuracy as they digest more information. Natural language processing (NLP) is super important in the world of AI-driven drug repurposing because it helps AI systems sift through the enormous amount of scientific literature out there. This includes everything from research papers and clinical trial reports to patent documents, all of which hold valuable insights about drug properties and their effects on diseases. With NLP algorithms, these documents can be scanned to pull out relevant information about how drugs work, the types of cancer involved, and the results of experiments. This knowledge is then woven into the AI model, allowing these systems to keep their predictions up to date with the latest research [7]. This way, the efforts to repurpose drugs are always based on the most current understanding of both the drugs themselves and cancer biology.

Another crucial technique is predictive modeling, which involves creating computational models that can forecast the outcomes of different drug interventions. When it comes to cancer, these predictive models can simulate how existing drugs might perform in various tumor microenvironments. They take into account factors like how drugs are absorbed, distributed, metabolized, and excreted. By analyzing genetic profiles, cancer mutations, and even specific patient factors, these models can predict the chances of success for drug candidates. This makes it possible to tailor drug repurposing efforts and potentially match treatments to the right patients more efficiently. Together, these AI techniques form a strong system that really boosts the drug repurposing process. By tapping into extensive datasets and advanced computational tools, AI can uncover new therapeutic uses for existing drugs that haven't been explored before, opening up exciting possibilities for cancer treatment [8]. As AI keeps advancing, its ability to sift through complex data, predict how drugs interact, and fine-tune treatment strategies will surely speed up the discovery of effective cancer therapies, ultimately enhancing patient outcomes and reshaping the field of oncology.

5. Key Steps in AI-Driven Drug Repurposing for Oncology

The journey of using AI for drug repurposing in oncology is quite fascinating and involves several important steps. It takes a mountain of biological and clinical data and turns it into actionable insights, ultimately helping to pinpoint and test existing medications for new cancer treatments. The effectiveness of this method hinges on blending cutting-edge AI technologies with a solid grasp of cancer biology, pharmacology, and the ins and outs of clinical trials. Every step, from gathering data to conducting trials, is vital in ensuring that repurposed drugs are both safe and effective for treating cancer. The very first step in this AI-driven drug repurposing adventure is data collection. To find the right candidates for repurposing, AI systems need access to extensive datasets that cover a wide range of areas. Molecular and genetic data, like genomic sequencing results, are crucial as they help AI algorithms grasp the specific mutations, gene expressions, and molecular pathways that change in cancer cells. Additionally, proteomics and transcriptomics data, which provide insights into protein functions and gene activity, further illuminate the biological mechanisms at play in cancer. On top of that, clinical data—such as patient demographics, treatment outcomes, and any adverse events—are key to understanding how different types of cancer respond to various treatments [9]. Plus, information about existing drugs, including their chemical structures, how they work, side effects, and past clinical results, is woven into the system. AI taps into this rich pool of data to predict how certain drugs might impact cancer cells or the tumor microenvironment, laying the groundwork for spotting potential repurposing candidates.

Once we've gathered all the relevant data, we move on to the exciting phase of drug discovery, where AI really shines in pinpointing potential candidates for repurposing. By using predictive algorithms, AI dives into the collected data to find drugs that might work against specific types of cancer. These algorithms evaluate how a drug interacts with various molecular targets linked to cancer, like mutated genes, signaling pathways, and tumor suppressors. AI models often employ deep learning techniques to analyze the molecular structures of drugs and align them with cancer-specific targets, predicting how effective they might be based on the biology of the disease. Additionally, machine learning algorithms can spot patterns and connections between drug features and cancer types, aiding in the discovery of drugs that weren't initially designed for cancer but could provide therapeutic benefits when repurposed [10]. This predictive capability speeds up the drug discovery process, enabling researchers to quickly focus on a shortlist of candidate drugs that deserve further exploration in cancer treatment. The next phase in the journey of AI-driven drug repurposing is all about validation and optimization. Once AI has pointed out potential candidates for repurposing, these drugs must undergo testing in lab models and eventually in clinical environments. But AI doesn't just stop at making predictions; it can also assist in designing and fine-tuning laboratory experiments to confirm how effective the suggested drugs really are. During preclinical testing, AI can pinpoint the most relevant experimental models, like specific cancer cell lines, animal models, or organoids that closely resemble the tumor biology we're interested in. Additionally, AI can help optimize dosages and treatment schedules, ensuring that these repurposed drugs are tested under conditions that reflect real clinical scenarios. In this phase, AI's role goes beyond just confirming the predicted activity of the drugs; it also helps identify the best combinations or treatment plans that could enhance effectiveness or lessen toxicity. Thanks to AI's knack for simulating complex biological interactions, we can take a more efficient and targeted approach to testing, reducing the number of experimental iterations needed to find promising candidates. Once a drug has proven effective in lab tests, the next hurdle is moving on to clinical trials. This phase can be quite lengthy, expensive, and filled with uncertainties. However, AI has the potential to speed up the clinical trial process for repurposed drugs, tackling some of the inefficiencies that have long been a part of traditional clinical development. For instance, AI can make the recruitment process smoother by pinpointing patient groups that are most likely to benefit from the repurposed drug, using insights from genetic markers, tumor characteristics, and previous treatment histories. This focused approach to selecting patients can help cut down trial costs and ensure that the clinical study is robust enough to yield meaningful results [11].

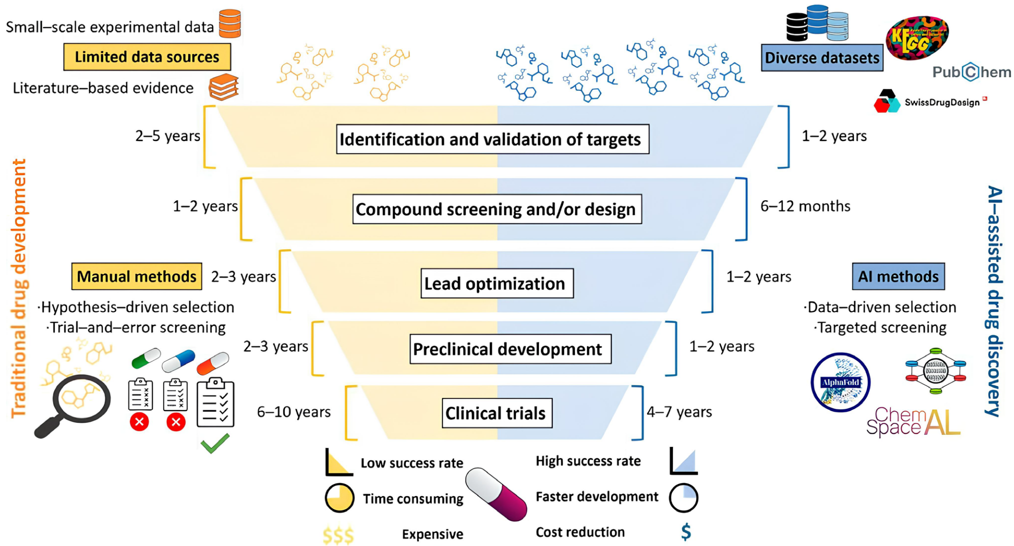

Figure 2. This images shows the key steps in AI-driven drug repurposing in oncology.

The contrast between traditional drug development and that done with AI assistance is displayed in **Figure 2**. The traditional side uses very limited data, relies on human hypothesis-driven selection, and subjects the drug development to massive trial-and-error processes over very long periods, even reaching ten years, at enormous expenses, and mostly producing failed results. On the other hand, AI methods source massive volumes of diverse data from public databases like PubChem and DrugBank for the automation and acceleration of all stages-target identification, compound screening, optimization, and preclinical development-reducing development time and costs while increasing success rates. The funnel shape illustrates the narrowing of potential candidates through each phase, with

AI streamlining this progression for faster, more efficient outcomes.

Moreover, AI can assist in refining trial designs by predicting the most effective dosages, treatment plans, and endpoints based on insights from earlier studies. Additionally, AI tools can monitor real-time data during clinical trials, quickly identifying any adverse reactions or unexpected responses, which allows researchers to make necessary adjustments on the fly. By automating data analysis, AI can significantly accelerate the evaluation of clinical trial outcomes, leading to quicker decision-making and a more streamlined path to regulatory approval. Throughout each stage—data collection, drug discovery, validation and optimization, and clinical trials—AI enhances the drug repurposing process, making it faster, more precise, and cost-effective. Integrating AI into drug repurposing for cancer treatment not only speeds up the discovery of new therapies but also allows for more personalized and targeted approaches to cancer care [12]. The ultimate aim is to bring effective and safe repurposed drugs to market more efficiently, providing innovative treatments to cancer patients in a fraction of the time it would take through traditional drug development. As AI continues to advance, its influence in transforming the drug repurposing landscape will only grow, paving the way for exciting breakthroughs in cancer treatment.

6. Harnessing the Power of Advanced AI Architectures in Drug Repurposing for Oncology

The real beauty of AI for drug repurposing in oncology is demonstrated in its ampleness and ability of the underlying complexity behind algorithms to not fully sound like a black-box solution from point A to point B. This approach is instead dependent on the ever dynamic interplay of machine learning and deep learning models that are born specifically to make sense of the biological systems and pharmacological datasets. Such methods include supervised or unsupervised learning techniques that process structured datasets gene expression profiles, protein-protein interaction networks, and drug response matrices to discover and identify latent patterns signifying possible therapeutic relevance towards a cancer-specific indication. Support Vector Machines (SVMs), Random Forests, and many gradient boosting frameworks such as XGBoost are usually utilized in the initial predictive models. They are especially useful in dealing with genomic data which is high dimensional in nature and is highly generalizable and robust against overfitting with proper feature selection done. They are particularly good in a scenario like this, trying to predict whether a drug would lead to an inhibition of the proliferation of a certain cancer cell line. However, non-linear and hierarchical relationships are not well-captured by it without giving plenty of engineered features, which proves a limiting factor in complicated biological interactions.

To defy that, deep learning architectures-mainly convolutional neural networks (CNNs), recurrent neural networks (RNNs), and even more recently, transformer-based architectures-were largely employed. CNNs have been proven effective in biomedical imaging and the 2D representation of molecules as with drugs and cell morphologies, looking for spatial features that could prove correlated with efficacy. By contrast, RNNs and long short-term memory networks (LSTMs) are designed specifically for the analysis of sequential biological data, such as DNA or protein sequences, and may be able to discover dependencies otherwise invisible to static models. With temporal models, it's also possible to address an area such as changes in patterns of gene expression induced by drug exposure over time. For the >90% of the molecule in the protein target, it is in a more functionally implemented manner in a GNN, which is another breakthrough in this arena, feasibly representing the molecular structures, biological pathways, and the heterogeneous drug-disease-target interaction networks. At this foundation, by learning from graph-structured data, GNN can encode complex relationships between entities such as shared targets between drugs or functional links between genes, effectively allowing for the discovery of mechanistically plausible repurposing candidates. Trained on suitable industrial knowledge graphs, GNNs have also been successful in drug prioritization for rare cancers where little experimental data can be obtained. Unlike GNNs, transformers were formerly applied to natural language processing but are adapted towards the more recent biomedical applications. Models like BioBERT and ChemBERTa learn rich contextual embeddings of biomedical literature and molecular sequences, respectively. These embeddings can be later fused with structured datasets to augment the prediction model and allow AI systems to infer drug-cancer associations even with very limited experimental knowledge.

Nevertheless, these deep learning models do have shortcomings. They need huge amounts of training data, demand enormous amounts of computational resources, and are in some cases not interpretable, thus posing a hurdle for regulatory acceptance and clinical trust. Research is being conducted to tackle such hurdles by the means of explainable artificial intelligence (XAI), providing transparency to the decision-making processes used by these complex models by identifying the most influential features or substructures in a given prediction. Furthermore, there has been an increasing prevalence of multi-modal models that incorporate different types of data-such as genomics, imaging, electronic health records, and scientific literature-producing a comprehensive view of the cancer landscape while enhancing predictive accuracy through cross-domain interaction capturing. However, harmonization and preprocessing of such significantly diverse data streams remain outstanding challenges requiring standardized frameworks and advanced pipelines for data integration. To sum up, AI drug repurposing for oncology is much more than the application of dull predictive analytics. This is a complex, evolving field, which combines statistical learning with biologically inspired architectures to investigate the therapeutic potential of known drugs in new cancer contexts. As algorithmic transparency, data access, and computational power improve, AI's importance in reshaping cancer treatment strategies will only strengthen, therefore leading to faster, better, and more potent drug discovery pipelines.

7. Challenges in AI-Driven Drug Repurposing

AI-driven drug repurposing in oncology holds incredible promise, but there are quite a few hurdles we need to jump over to unlock its full potential. From the quality and accessibility of data to the intricate nature of molecular mechanisms and the regulatory challenges, these issues require thoughtful consideration and creative solutions to ensure that AI can truly revolutionize cancer treatment. Each of these challenges is a vital piece of the puzzle that can impact the success of AI in drug repurposing, making it crucial for researchers, healthcare professionals, and regulatory agencies to collaborate in tackling them. One of the biggest hurdles in AI-driven drug repurposing is the quality and availability of data. Having high-quality, well-annotated datasets is essential for training AI models that can accurately predict how effective and safe a drug might be. However, the data that AI systems rely on often comes from a mix of sources, including genomic, clinical, proteomic, and drug-related information, each presenting its own set of challenges [13]. For instance, genomic data can be incomplete, noisy, or inconsistent across different patient groups, which can introduce biases into AI models. Likewise, clinical data might have inconsistencies due to variations in how patient outcomes are documented or how treatments are given. Issues with data quality, like missing values, inaccuracies, or a lack of standardized formats, can seriously hinder AI systems' ability to make trustworthy predictions. Plus, while large datasets are incredibly useful, they aren't always available for every type of cancer, especially for rarer ones where clinical trial data or molecular research might be scarce. Without access to high-quality, comprehensive datasets, AI's capacity to pinpoint promising drug repurposing candidates and forecast their effectiveness in specific cancer types is significantly restricted [14].

One of the big hurdles we face is the intricate challenge of figuring out how repurposed drugs actually work in cancer therapy. Sure, AI might be able to predict which drugs could be effective for certain types of cancer, but grasping the specific molecular mechanisms behind these effects is a whole different ball game. Cancer is incredibly diverse, with a multitude of genetic mutations, signaling pathways, and environmental factors all playing a role in how tumors grow and spread. A medication that works wonders for one patient might not do a thing for another, simply because of the unique molecular makeup of their cancer. Repurposed drugs, which weren't originally created to fight cancer, often interact in complex ways with various pathways in the body. To truly understand how a drug might impact cancer cells and how it could work alongside other treatments, we need to dive deep into these interactions [15]. While AI can certainly help by sifting through massive amounts of biological and clinical data to predict these interactions, it still doesn't quite capture the subtle nuances of cellular processes that come from hands-on biological experimentation. The real challenge lies not just in spotting a potential drug but also in comprehending how it operates at a molecular level, which is essential for fine-tuning treatment plans and reducing side effects. Navigating the regulatory and ethical landscape is a major challenge in the world of AI-driven drug repurposing. Getting regulatory approval for a repurposed drug, even one that's already been tested for other uses, can be quite a complex and lengthy process. Agencies like the U.S. Food and Drug Administration (FDA) and the European Medicines Agency (EMA) demand solid evidence of safety and effectiveness before they'll greenlight a drug for new uses. While repurposed drugs might have a proven safety record, their effectiveness in treating cancer still needs thorough evaluation through clinical trials specifically designed for the type of cancer in question. On top of that, the role of AI in drug repurposing raises fresh concerns about accountability and transparency [16].

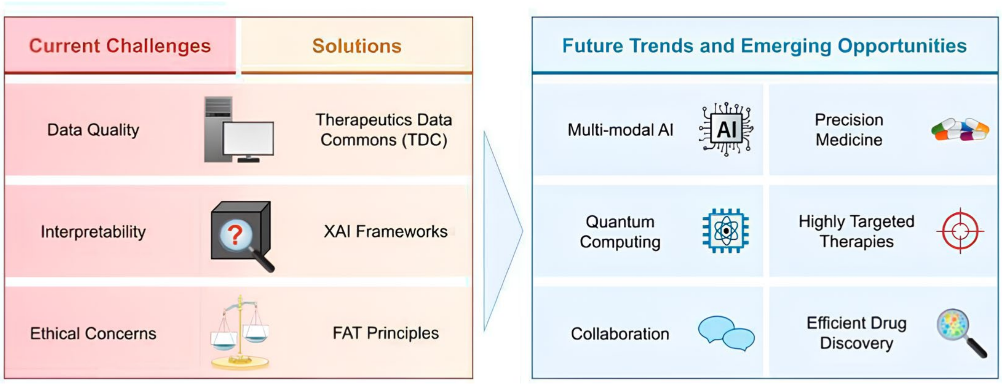

Figure 3. This image shows the challenges in AI drug repurposing.

Figure 3 brings out the transformation in the current woes of AI-supported drug discovery to some opportunities that sit on the horizon. Challenges include data quality, interpretability, and ethics. In turn, solutions include the Therapeutics Data Commons (TDC) for standard data, an Explainable AI (XAI) framework for transparency, and Fairness, Accountability, and Transparency (FAT) principles for ethical considerations. All of these areas set the stage for upcoming trends, such as multi-modal AI pulling together different types of data; quantum computing tackling complex issues; collaborative ecosystems, precision medicine; precision-targeting therapies; and improved drug discovery pipeline efficiency. This begs the question: the dawn of a truly intelligent, ethical, scalable pharmaceutical paradigm?

AI models, especially those based on deep learning, are often viewed as "black boxes" because their decision-making processes can be hard to decipher. This lack of clarity makes it tough to convince regulatory bodies, healthcare professionals, and patients that the predictions from AI systems are reliable and valid. Moreover, we need to carefully address ethical issues related to AI in medicine, such as data privacy, informed consent, and algorithmic bias. It's crucial to ensure that AI models don't perpetuate existing health disparities or unintentionally leave out certain patient groups, as maintaining ethical standards in drug repurposing is essential. Integrating AI into the traditional drug development process presents quite a challenge. Many pharmaceutical companies, clinical researchers, and healthcare professionals are used to tried-and-true methods of drug development, which can make them hesitant to embrace change. Approaches driven by AI, which depend on extensive datasets and predictive modeling, might be met with skepticism or seen as just another complication instead of a valuable tool. To overcome this resistance, we need a shift in perspective—AI should be viewed not as a replacement for human expertise but as a way to enhance and support it. For AI predictions to truly fit into clinical practice, there needs to be a partnership between AI specialists and oncologists, ensuring that the predictions from AI models are scientifically sound and relevant to real-world clinical situations. It's essential that AI models can be smoothly integrated into existing workflows, giving clinicians actionable insights that can enhance patient care. Moreover, healthcare providers need training to interpret AI predictions and weave them into treatment plans, which involves both technical know-how and trust in the technology. The real potential of AI shines through when it's seamlessly woven into the decision-making processes that shape patient care, ensuring it boosts rather than disrupts traditional clinical expertise [17]. In short, while AI-driven drug repurposing for oncology shows great promise, it comes with its own set of challenges. We need to ensure high-quality data is available, grasp the complex mechanisms of drug actions, navigate regulatory and ethical issues, and tackle the resistance to incorporating AI into established workflows. By addressing these hurdles, we can unlock the full potential of AI in revolutionizing cancer treatment, paving the way for faster, more efficient, and personalized therapeutic options for patients.

8. Navigating the Challenges and Ethical Complexities of AI-Driven Drug Repurposing

AI-driven drug repurposing does provide a much-needed path for a revolutionized approach towards hastened discoveries in cancer remedy development; however, this path is fraught with enormous challenges. The realization of this promise exists in an intricate landscape of limitations that have to be surmounted in order to actually translate computational foresight into the arena of therapeutic fact. One of the major problems, which one could therefore say is a perennial one, lies in data bias—an inevitable pitfall during model training due to incomplete and highly unbalanced biomedical datasets skewed toward certain populations, diseases, or treatment outcomes. For example, genomic databases and clinical trial repositories tend to under-specify minority groups, rare cancer subtypes, and long-term treatment data—all factors that lead to having models that may not successfully generalize over diverse patient populations. The influences that these biases set in would not be overt but gradually infiltrate the predictions, all leading to erroneous conclusions regarding drug efficacy or safety. The constraints that certain models face for under-represented tumor types or treatment responses make them overfit to patterns that may have no clinical or biological robustness upon which to base generalizing conclusions. This is a major concern within oncology, as any decision supported by biased data would become a matter of life and death. Biases thus require the establishment and standardization of model training, data collection processes, and inclusion criteria in biomedical research, alongside the application of bias-detection tools during model development. Another concern is interpretability of the model. Most of the deep learning architectures applied in drug repurposing have a high degree of accuracy but operate as black boxes with very little information on how a particular prediction was made. The stakes become high for clinicians and regulators needing to evaluate the rationale for AI-based suggestions. Currently, there is research being developed toward the goal of integrating explainability into these systems, with techniques that attempt to highlight which genomic features, drug properties, or clinical variables trigger a model's decision. Interpretability still has a long way to go, especially with models becoming increasingly complex and multi-modal.

Ethics is an area that further complicates the use of AI in oncology drug discovery. Decisions from these models bear an immediate impact on patient health, creating the moral obligation that one should ensure those predictions are indeed technically correct and socially responsible. Questions such as data privacy, informed consent, and willful misuse of predictive insights are evermore pressing as AI systems are already scanning into personal health records, genetic information, and real-time clinical data. The consideration of algorithmic harm, however that be through negligence, oversight, or willful misuse, emphasizes the necessity for extremely strong ethical governance frameworks and a patient-centered approach. In reality, no matter how advanced, any computational estimation is subject to irrefutable validation by clinical testing. The biological complexity of cancer can therefore never be completely reflected in silicon; what looks good on a computer might collapse in the subtle milieu of the human body. Clinical trials are the gold standard for proving the safety and efficiency of any therapeutic plan, AI-induced or otherwise. Fast turnarounds and reduced cost should never be made at the price of scientific integrity. The FDA and EMA are beginning their quest for outlining pathways for the assessment of AI-related drug design, yet those frameworks are still in development, calling for collaborative case studies from disparate fields: data scientists, normative oncologists, ethicists, and regulators. In the long run, some balance must be reached between AI re-purpose in oncology applications and ethical principles. The rapid enthusiasm of a very innovative process must meet critical equal concerns of transparency, fairness, and patient safety. The very challenges posed by data quality, model bias, interpretability, and clinical validation are not technical obstacles; they are the very prerequisites to the establishment of truly better systems that will enhance cancer care. These challenges will mature into an opportunity for the design of stronger, ethical, and accountable frameworks of AI that impact not only the science of oncology but also the lives of patients it intends to benefit.

9. Potential Benefits and Impact on Oncology

The use of AI in drug repurposing for cancer treatment has the potential to revolutionize how we approach oncology. It brings a host of benefits compared to the traditional drug development process. By quickly identifying existing medications that could be effective against cancer, we're making a significant stride in medical research, paving the way for faster and more cost-efficient drug development. We all know that traditional drug discovery can be a long and costly journey, often taking years or even decades to move a new cancer drug from the lab to the clinic. This process is not only slow but also comes with a high risk of failure during clinical trials, which drives up costs even more. However, by harnessing AI to repurpose drugs that are already on the market, researchers can bypass much of the early development stages, like initial safety tests and pharmacological assessments, since these drugs have already been rigorously tested in humans for other conditions. This more efficient approach significantly cuts down both the time and money needed to develop new cancer treatments, ultimately making them more accessible and affordable for patients.

One of the most significant advantages of using AI for drug repurposing in oncology is its ability to boost personalized medicine. Cancer is incredibly diverse, with each patient's tumors often showing distinct genetic, molecular, and environmental traits. This variety makes it tough to find treatments that work for everyone. However, with AI, we can customize repurposed drugs to fit specific cancer subtypes, considering factors like genetic mutations, the tumor microenvironment, and how cancer cells respond to different treatments. AI can analyze massive datasets to pinpoint repurposed drugs that might be effective for individual patients based on their unique cancer profiles. This tailored approach not only raises the chances of successful treatment but also reduces the risk of unnecessary side effects, which is vital for enhancing the quality of life for those battling cancer. Another important benefit of AI-driven drug repurposing is the potential for better patient outcomes. Traditional cancer therapies, such as chemotherapy, immunotherapy, and radiation, often come with serious side effects like fatigue, nausea, and organ toxicity, which can greatly impact a patient's well-being and overall outlook. In contrast, repurposed drugs might provide a milder option with fewer side effects, especially when they are already established medications with known safety records [18]. AI can help discover drugs that, although initially created for other conditions, may effectively target cancer cells while sparing healthy tissue. These repurposed therapies could lead to improved patient tolerance and adherence to treatment plans, ultimately enhancing survival rates and the quality of life for cancer patients.

Figure 4 depicts how artificial intelligence (AI) helps to level up cancer management under three major concepts. AI can analyze patient data on a big scale to create individual treatments, which may lead to more effective therapies. It also enhances the accuracy of cancer diagnosis by reducing false positives and false negatives, allowing for less chance of misdiagnosis of patients. To add to that, AI is enabling minimally invasive procedures to diagnose and treat cancers, thus reducing patient discomfort and risk during their management.

Figure 4. This image shows the benefits of AI in oncology.

AI-driven drug repurposing could really change the game when it comes to cutting down healthcare costs. The usual route of creating new cancer drugs from scratch is not just pricey; it also comes with a lot of risks. Many promising drugs that look good in the lab end up failing during later clinical trials, which leads to wasted money from all those failed studies. By shifting the focus to repurposing drugs that have already been proven safe for humans, AI can help minimize the chances of failure and cut down on the expensive clinical trials needed to get a drug approved. This means healthcare systems can roll out new treatments faster, giving patients more timely options while also slashing the costs tied to lengthy drug development processes. The possibility of quicker approvals and lower failure rates means that more drugs can be tested at the same time, speeding up the discovery of effective treatments for different cancer types and patient groups. This could ease the financial strain on healthcare systems and ultimately make cutting-edge cancer therapies more accessible to patients around the globe. In short, AI-driven drug repurposing has the potential to significantly impact oncology by accelerating the drug development process, lowering costs, and offering more effective, personalized treatment options. By providing patients with new therapies that have fewer side effects and better outcomes, this approach not only promises to enhance cancer care but also aims to make it more sustainable and accessible. The ongoing advancements in AI technology, paired with the vast amount of existing drug data, could truly revolutionize cancer treatment, making the battle against cancer faster, smarter, and more effective [19].

10. Case Studies and Recent Successes

AI-driven drug repurposing in oncology is making waves, showcasing its incredible potential through various success stories where existing medications are being tested for new cancer applications. These examples illustrate how AI can speed up the identification of effective treatments for different types of cancer by tapping into a wealth of data from various sources, such as molecular profiles, patient histories, and existing drug information. With the help of sophisticated AI algorithms, researchers are uncovering unconventional drug candidates that were initially created for other diseases, revealing their hidden potential in cancer therapy. One standout success story is the repurposing of the antimalarial drug chloroquine for cancer treatment. Initially designed to combat malaria, chloroquine has shown promise in fighting cancer due to its ability to inhibit autophagy—a cellular process that some cancer cells depend on to thrive in tough conditions, like when nutrients are scarce. While chloroquine was already recognized for its anti-inflammatory and immunomodulatory properties, it was AI's knack for sifting through massive genetic and molecular datasets that pinpointed it as a viable candidate for cancer therapy. AI models, trained on genomic data and cancer cell behavior, suggested that chloroquine could effectively disrupt tumor cell growth, especially in cancers like glioblastoma. This revelation paved the way for clinical trials, where chloroquine, sometimes paired with other drugs, was tested on patients with specific cancer types. The results showed that chloroquine could be repurposed as a complementary treatment, boosting the effectiveness of other cancer therapies and potentially leading to better outcomes for patients. One fascinating example is the antibiotic doxycycline. Initially created to tackle bacterial infections, it was later discovered by AI to have the potential to slow down cancer cell metastasis. By analyzing molecular data and patient treatment results, AI pinpointed doxycycline as a drug with unexpected effects that could influence cancer progression [20]. It turns out that doxycycline can inhibit the enzymes that cancer cells rely on to invade nearby tissues, which is a crucial step in the metastatic process. In clinical trials, doxycycline has shown real promise, especially for cancers that have a high risk of spreading, like lung and breast cancer. This highlights how AI can play a vital role in identifying drugs for new purposes, showcasing its ability to go beyond traditional drug categories and find innovative uses in oncology. (**Figure 5**)

It could display a case study for AI in drug discovery and how much faster machine learning algorithms analyze vast biological data for identifying possible drug candidates than traditional methods. Faster by predicting molecular interactions, time savings may reduce a process from years to months and cost savings too. The application could also indicate successful application resulting from AI development of a new compound against a particular disease thereby demonstrating a greater efficacy of repurposing existing drugs into new therapies. Overall, it portrays how AI is revolutionizing drug discovery as smarter, faster, and more targeted.

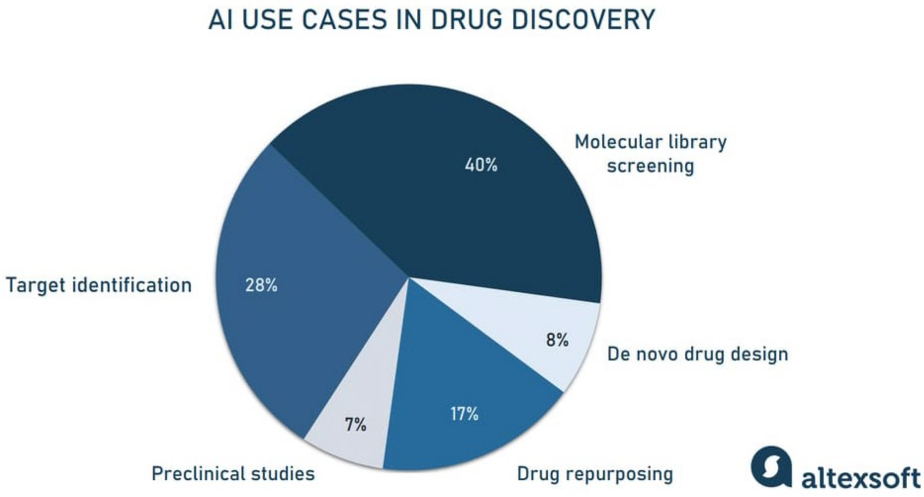

Figure 5. This image shows the case study of AI use in drug discovery.

Another impressive success story driven by AI is the repurposing of the antidepressant fluoxetine, commonly known as Prozac, for cancer treatment. Fluoxetine, a popular selective serotonin reuptake inhibitor (SSRI) used for depression, was examined using AI algorithms that analyzed data from cancer genomics and patient outcomes. AI proposed that fluoxetine might possess anti-cancer properties by influencing cancer cell survival pathways and boosting the body's immune response to tumors. In lab experiments, fluoxetine showed it could inhibit the growth of certain cancers, including pancreatic cancer, which is notoriously tough to treat. Additionally, AI discovered that fluoxetine could enhance the effectiveness of chemotherapy by making tumor cells more sensitive to treatment. This finding is significant because it not only provides a new treatment option for pancreatic cancer patients but also illustrates how AI can uncover surprising new uses for drugs that were never originally intended for cancer therapy. In a recent breakthrough, researchers harnessed the power of AI to pinpoint existing medications that could be used to treat glioblastoma, a particularly aggressive and challenging brain cancer. They employed AI models to sift through vast amounts of genetic and clinical data from glioblastoma patients, examining everything from mutations and gene expression profiles to how patients responded to various drugs. The AI system successfully identified several medications that had been previously used for other ailments, including some that were tested for neurological disorders. Remarkably, these drugs showed potential effectiveness against glioblastoma by targeting specific mutations or interfering with the pathways that fuel tumor growth [21]. This discovery has sparked the launch of clinical trials to investigate the use of these repurposed drugs for glioblastoma treatment, bringing a glimmer of hope to patients who have limited options.

These success stories highlight the incredible promise of AI-driven drug repurposing in oncology, where existing FDA-approved medications can be re-evaluated for their potential in treating different types of cancer. AI not only speeds up the process of finding promising drug candidates but also helps determine which drugs should be prioritized for testing in clinical trials based on their molecular characteristics and past usage data. By utilizing AI for drug repurposing, we can significantly cut down the time and costs typically involved in drug discovery, while also paving the way for new cancer treatment possibilities. As AI algorithms continue to evolve and datasets expand in size and detail, the chances of uncovering innovative cancer therapies will only grow, offering renewed hope for patients facing limited treatment options. These examples highlight the incredible impact AI is having on the way we approach cancer treatment. By leveraging smart data analysis and predictive modeling, AI is discovering new uses for existing medications, speeding up the process of getting promising therapies to patients, and ultimately enhancing cancer care with innovative, targeted, and potentially less harmful treatments.

11. Future Directions and Potential Developments

The future of using AI for drug repurposing in oncology is looking really promising. As artificial intelligence keeps advancing, it's making significant strides in personalized cancer therapy. AI is set to become a key player in customizing treatments to meet the unique needs of each patient, pushing the boundaries of precision medicine. With cancer treatments becoming more tailored, AI will be essential in sifting through massive amounts of data—like genomic, molecular, and clinical information—to uncover the most effective and least harmful therapies for individual patients. By considering the distinct genetic profile of a patient's tumor and its surrounding environment, AI can pinpoint repurposed drugs that are ideally suited for that specific type of cancer. As AI algorithms get smarter, they won't just help in choosing the best repurposed treatments; they'll also enable continuous monitoring and adjustments to treatment plans based on real-time patient data, ultimately enhancing outcomes and reducing side effects [22]. This personalized strategy has the potential to transform how oncologists approach cancer treatment, ensuring that therapies are tailored not only to the type of cancer but also to the unique molecular features of each patient's condition. As AI continues to evolve in the realm of personalized cancer therapy, new technologies and tools are stepping up to boost the potential of AI-driven drug repurposing. With advancements in machine learning algorithms—especially deep learning and reinforcement learning—we can expect even better predictive accuracy from AI systems. This means they'll be able to handle and analyze larger, more complex datasets than ever before. As these algorithms get smarter, they'll start to reveal subtle patterns in cancer biology that traditional methods might overlook. Natural language processing (NLP) is another exciting area that's set to grow, helping to sift through the massive amounts of unstructured data found in scientific literature, clinical trial reports, and electronic health records. By leveraging NLP, AI can uncover fresh insights into how existing drugs interact with cancer cells and spot new opportunities for drug repurposing. Plus, we're likely to see AI teaming up with other cutting-edge technologies like CRISPR gene editing and organ-on-a-chip models. These partnerships will lead to more accurate in vitro and in vivo testing systems, simulating the human body in ways that older models simply can't. This means we'll be able to make better predictions about how repurposed drugs will perform in patients. All these advancements will help researchers pinpoint effective drug candidates faster, ultimately speeding up the process of getting new treatments to market [23].

Looking ahead, the future of AI-driven drug repurposing in oncology is set to thrive through enhanced collaboration among AI researchers, oncologists, and pharmaceutical companies. To truly unlock the potential of AI in this field, it's essential for everyone involved to come together. Oncologists bring invaluable clinical expertise and patient insights that help make sense of AI predictions and apply them effectively in treatment plans. Meanwhile, pharmaceutical companies contribute their understanding of drug development processes and regulatory standards, ensuring that any repurposed drugs are safe and effective. By working hand in hand, AI researchers, oncologists, and the pharmaceutical industry can speed up the discovery and implementation of repurposed drugs. These collaborative efforts will lead to the creation of richer datasets, improved AI algorithms, and more focused clinical trials. Such partnerships will also make it easier to weave AI into the daily clinical workflow, allowing clinicians to integrate AI insights into their decision-making seamlessly. As these collaborative networks grow, they'll help tackle some of the hurdles to widespread AI adoption, like worries about data privacy, transparency in algorithms, and how to incorporate AI predictions into clinical practice. We also need to address ethical considerations, ensuring that AI technologies are used equitably in healthcare so that all patients can benefit from these advancements. By confronting these challenges directly, we can make sure that AI-driven methods become a standard part of oncology practice, paving the way for more accessible and effective personalized cancer treatments. The merging of AI with cutting-edge technologies, along with ongoing teamwork across various fields, is set to usher in a groundbreaking era in cancer treatment. Imagine a world where drugs that have already been deemed safe can be quickly and effectively repurposed for new cancer uses. This approach is bound to uncover innovative therapies that are not only more precise and less harmful but also customized for each patient [24]. The ultimate goal? To enhance survival rates and improve the quality of life for those battling cancer. With these exciting developments on the horizon, AI-driven drug repurposing in oncology is poised to revolutionize cancer care, bringing fresh hope to patients and paving the way for more effective and efficient treatments in the future.

12. Conclusions

AI-driven drug repurposing is a game changer in the world of oncology, opening up exciting new paths for treatment by pinpointing existing medications that might work against cancer. By tapping into a wealth of data—from molecular and genetic information to clinical insights—AI can uncover drug candidates that might have been missed before, significantly cutting down the time and costs typically involved in traditional drug development. But the potential of AI in oncology goes beyond just speeding up the discovery of new therapies. It also allows for a more personalized approach to cancer treatment by matching repurposed drugs with specific cancer subtypes, which can lead to more effective and less toxic therapies. This means we could improve patient outcomes while minimizing side effects and lowering healthcare costs, marking a major advancement in the battle against cancer. That said, the path to fully harnessing the power of AI-driven drug repurposing is fraught with challenges. We still face issues like data quality, the intricate nature of cancer biology, and the need to integrate AI technologies into existing clinical practices. Plus, we have to navigate regulatory and ethical concerns to ensure that these AI-driven methods are implemented safely and fairly. Tackling these challenges will take ongoing research, collaboration, and innovation across various fields, including AI development, oncology, and the pharmaceutical industry. Only by committing to these efforts can we truly unlock the potential of AI-driven drug repurposing.

Looking ahead, it's clear that the future of cancer treatment is becoming more and more connected to the exciting advancements in AI and drug repurposing. As AI technology evolves and we gather more comprehensive datasets, the chances of uncovering innovative cancer therapies are set to increase. By working together, researchers, clinicians, and industry leaders can speed up the integration of AI into oncology, which means we'll see quicker identification of treatment options, more personalized care, and better outcomes for patients. The ongoing progress in AI-driven drug repurposing is incredibly promising, not just for improving existing cancer treatments but also for paving the way for new, targeted, and accessible therapies. With every step forward, AI is bringing us closer to a future where cancer is not only easier to manage but, in the end, more curable.

Conflicts of Interest

The authors declare no conflicts of interest regarding publication of this paper.

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