Drug Design, Development and Therapy

Dovepress
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REVIEW

Artificial Intelligence-Driven Innovations in Oncology Drug Discovery: Transforming Traditional Pipelines and Enhancing Drug Design

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Abstract: The integration of artificial intelligence (AI) into oncology drug discovery is redefining the traditional pipeline by accelerating discovery, optimizing drug efficacy, and minimizing toxicity. AI has enabled groundbreaking advancements in molecular modeling, simulation techniques, and the identification of novel compounds, including anti-tumor and antibodies, while elucidating mechanisms of drug toxicity. Additionally, AI has emerged as a critical tool in precision medicine, driving the formulation and release of targeted therapies and improving the development of treatments for oncology and central nervous system diseases. Furthermore, AI-assisted clinical trial designs have further optimized the recruitment and stratification of patients, reducing the time and cost of trials. Despite these advancements, challenges such as data integration, transparency, and ethical considerations persist. By synthesizing current innovations, this manuscript provides a comprehensive analysis of AI-driven approaches in drug discovery and their potential to advance oncology therapeutics and precision medicine. It examines the transformative role of AI across the drug development continuum, with a focus on its applications in computer-aided drug design (CADD), generative artificial intelligence (GAI), and high-throughput screening (HTS).

Keywords: artificial intelligence, oncology drug discovery, target identification, machine learning in oncology

Introduction

Since prehistory times, human endeavors to obtain medicines have been relentless, and these efforts have continued till the employment of modern technology to develop new medicines.[1] Conventionally, the development of a novel medicine lasts for a long time lasts around 12–15 years or longer until it is approved for marketing.[2] In addition to being time consuming, developing a novel drug is also financially burdensome reaching to 1–2.6 billion dollar.[3,4] Earlier in 1950 to about 1980, in vivo investigations were the primary source of data to develop new drugs.[5] Recently (1980s up to date), new technologies have been innovated to develop new drugs such as combinatorial technology, structure-based drug design, compound libraries, output of in vitro screening, and defined molecular targets. Yet, there is a remaining issue about launches of new drugs that have been reducing in the past two decades due to the increased complexity of drug research, and the issue of new safety requirements that brought unexpected obstacles for translating in vitro activity to in vivo one.[5]

Nowadays, computational sciences have been introduced in the field of developing and discovering new medicines to accelerate time and minimize cost, constituting the underlying driving motivation for employing artificial intelligence (AI) in the project of developing new medicines according to the clinical need as shown in (Figure 1).[2, 6]

A paramount branch of computational science is AI, which simulates human intelligence by computer systems. AI has become able to achieve several tasks of acquiring information, developing rules to utilize information, and self-correction,[6] based on algorithms.[7] An AI algorithm is a set of rules to make decisions about the acquired and utilized

Received: 2 December 2024
Accepted: 24 June 2025
Published: 3 July 2025

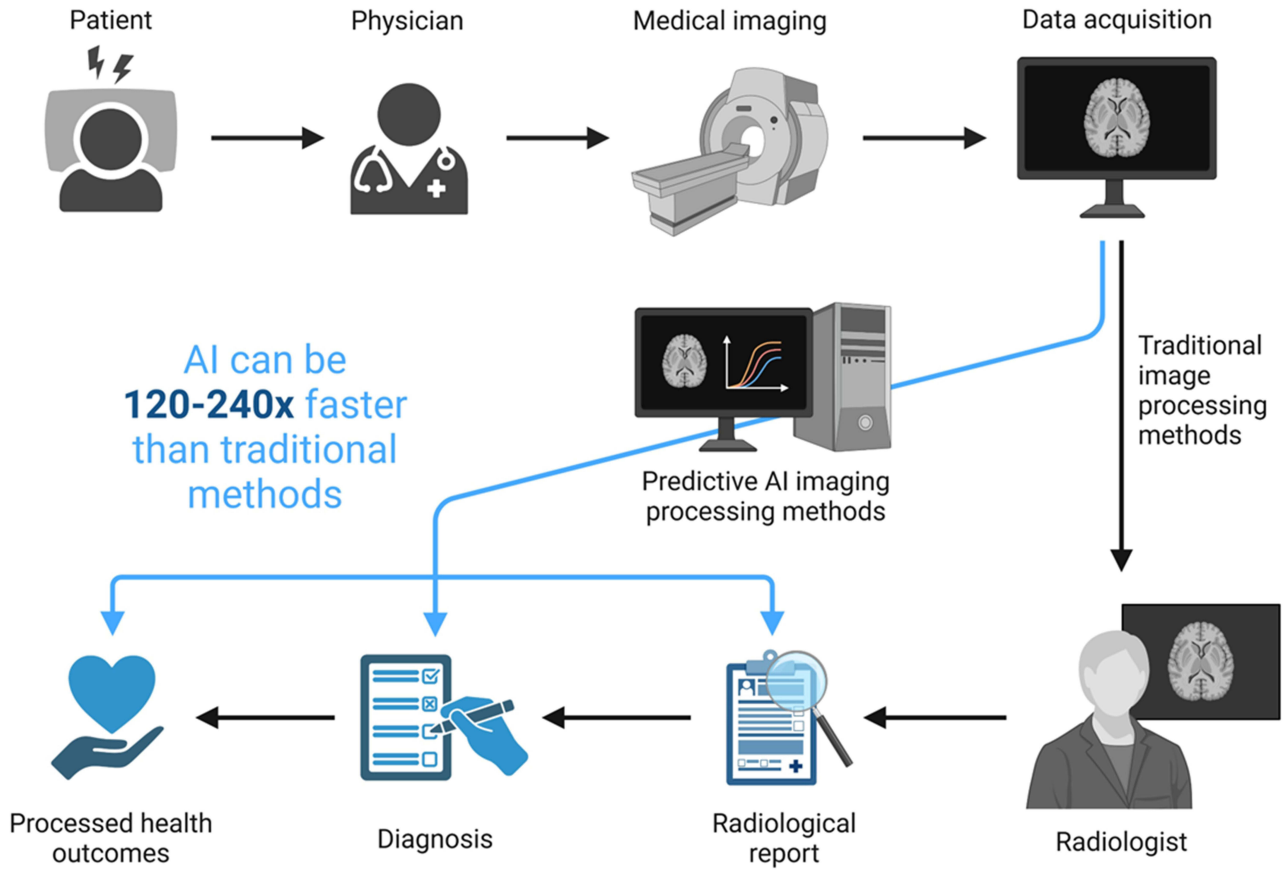

Figure 1 Biomedical image analysis (AI vs traditional techniques).
Notes: Created in BioRender. Ghanim, F. (2025) https://BioRender.com/hulhuw8.

data, requiring supervised input of data by human or unsupervised statistical methods.[7] AI algorithms appear to be promising in solving problems and overcoming obstacles faced with discovering and designing new drugs.[8] Thus, AI is a key driver of the transformation of health care to precision medicine.[9]

One of the AI applications is the drug development pipeline to discover new drugs by pharmaceuticals and academia[6,10] based on generating data to develop a hypothesis that proposes a therapeutic effect for the designed new medicine through inhibiting or activating a specific protein (eg, receptor, enzyme, structural protein) or signaling pathway.[2] Researchers can develop new medicines depending on creating a predictive model for the pharmacological activity and pharmacokinetic profile of the designed drug molecule, depending on the input and output of data.[6]

Several steps have been taken to develop a new medicine by AI. The first step is to design a drug molecule with a certain biological activity, which would arise from the interaction of such a designed drug molecule with a specific biological structure (receptor, protein, enzyme, nucleic acid, or gene). The second step is the identification of what is called "a lead molecule" that demonstrates a promising potential to develop a novel molecule to treat a certain disease. Once the lead molecule is discovered, a chemical structural modification is initiated to produce a molecule with maximal therapeutic benefit and minimal toxicity.[6] Thereafter, the outcome of the former steps requires further validation before being progressed into the discovery phase for justifying drug discovery efforts, candidate molecule will progress into preclinical studies (cell-based and animal-based studies). Thus, if this candidate molecule is successful, it will progress into clinical trials and ultimately be a marketed medicine.[2]

This study focuses on how AI is utilized to accelerate and optimize discovering and improving anti-tumor agents. This review highlights various applications in computer-aided drug design (CADD), generative artificial intelligence (GAI), and high-throughput screening (HTS) in the oncology field.

Target Identification

A drug target is versatile, including several biological entities (eg, receptors, enzymes, nucleic acids, structural proteins, transports),[2] which are specific sites on biomolecules in the body to which a drug binds to produce the desired therapeutic effect for treating or even preventing a specific disease.[11] Hence, target identification is a paramount step in developing a new medicine[2] The development of a new medicine relied in some cases on the principle of binding a single ingredient to one target for treating one disease due to the significant interference with target identification that would arise from a combination of the drug with multiple targets, yet, this would not be always the case.[12–14] The latter situation offers possibilities and opportunities for discovering and developing new drugs, particularly with natural products, which exert multiple effects due to the fact that these natural products are comprised of diverse chemical compounds with broad biological activities, and hence combine with multiple targets.[15,16] Therefore, the identification of targets of natural products (botanical bioactive) is fundamental to contribute in the optimization of existing drugs to accelerate the development of new drugs.[17,18] Nevertheless, there has been a bottleneck hindering the conduct of further research into applying natural products due to the fact that targets for several bioactive molecules are still unidentified.[19,20]

For target identification, data mining of available biomedical data is used, which significantly increases target identification. More specifically, data mining refers to the utilization of bioinformatics to assist in identifying, selecting, and prioritizing potential disease targets. Such data come from several sources, publications, and patent information in the literature, data on proteomics, gene expression, compound profiling, and transgenic phenotyping.[21]

For instance, since the outbreak of coronavirus disease 2019 (COVID-19), a huge number of investments by research institutions have been employed to develop and screen anti-COVID-19 drugs and vaccines with the assistance of data mining and bioinformatics to identify potential targets and drugs for preventing and treating COVID-19.[22]

Another example is brain metastasis (BM), which is a complication of triple-negative breast cancer (TNBC) due to the invasion of TNBC cells into the brain, and it is the most severe threat to patients' survival with TNBC. Unfortunately, the bottleneck is that no up-to-date drug has been approved for treating TNBC-derived BM (TNBCBM).[23] Despite huge efforts that have been made to discover a drug and druggable targets for treating TNBC-BM, the lack of targeted therapy, besides the high toxicity of the existing medicines and difficulties in delivering drugs to the brain are still key challenges for treating TNBC-BM.[24] Additionally, although a few drugs to treat TNBC-BM have progressed into clinical trials, and fewer have been approved for use compared to numerous molecular targets that have been identified to target TNBC-BM in terms of pharmacological molecular targets.[25]

Target Validation

Once the target is identified, a full prosecution of the target should be followed (ie, to be validated). The validation techniques for the prosecuted target go through in vitro and in vivo investigations for modulating a desired target in patients. Although target identification and validation are a multifunctional process and valid by their right, a multi-approach validation is required because it significantly increases confidence in the observed outcomes.[2] Thus, careful execution of target identification and validation is the cornerstone for reducing attrition rates to avoid poor efficacy. Additionally, the complementarity of phenotypic and target-based drug discovery methods would enable the discovery of first-in-class molecules, resulting in delivering more efficacious, safer and potent best-in-class follower molecules.[26]

Recent study closely associated to target identification and validation of drug discovery for treatment cancer[27] the researchers were used an AI-driven screening strategy to identify a new anticancer drug, Z29077885, that target STK33, the AI system included a large database combining public databases and manually curated information to describe therapeutic patterns between compounds and diseases. For target validation, they were used In vitro and In vivo studies to validate the Z29077885 as anticancer and they were investigated the mechanism of action by induce apoptosis by deactivation of the STAT3 signaling pathway and causes cell cycle arrest at S phase, and confirmed that treatment with Z29077885 decreased tumor size and induced necrotic areas. So, this study shows the efficacy of target in both in vitro and in vivo models. Moreover, this study confirms that successful use of AI-driven methods for target identification and validation in cancer drug discovery.

Stages in Drug Discovery

Identifying the medical need constitutes the motivation that stands behind drug discovery while considering whether the proposed hypothesis of therapy improvement in term of safety, efficacy, or mechanistically will influence the treatment for patients with the target disease through the developed or discovered therapy compared to the existing therapies. Setting the objectives, followed by employing the appropriate biological method to test the related chemicals is essential when answering the question correlated to the adequacy of the current agents.[5,26,28]

Key subsequent steps include a "hit" (in vitro detection of a relevant biological activity) for a structurally novel molecule, followed by preclinical investigation for the biological activity (in vivo investigation in a proper animal model). We then maximize the biological activity of the tested molecule through preparing structural analogues. Finally, selecting an analogue is to be the drug development candidate.[5,26,28] The toxicity of the drug candidate will be evaluated in a proper animal model. Passing all the preclinical investigations successfully, the accumulated data are gathered and submitted as the Investigational New Drug Application (IND) to the Food Drug Authorities (FDA) before being progressed into clinical trials.[5,26,28]

In the clinical trials, the candidate drug is progressed initially to Phase I clinical trial to evaluate toleration in normal human volunteers. Then, a further Phase II starts to assess efficacy and dose-escalation in patients with the target disease. Finally, Phase III is followed by widespread trials, involving a bigger sample size to develop a broad database for safety and efficacy.[5,26,28] Even if the drug candidates pass successfully the three phases of the clinical trials, a few drug candidates (4–7%) are submitted as IND, containing all research data to be reviewed by the experts at the FDA to approve the new medicine for clinical use as illustrated in (Figure 2).[5,26,28]

In the "R" discovery phase (research phase), a part of the hypotheses that constitute the project basis produced what is called "a drug candidate". In the "D" phase (drug development phase), approximately 1 out of 15–25 drug candidates pass efficacy and safety tests (in animals and humans) to be approved for marketing as summarized in (Figure 3).[5,29]

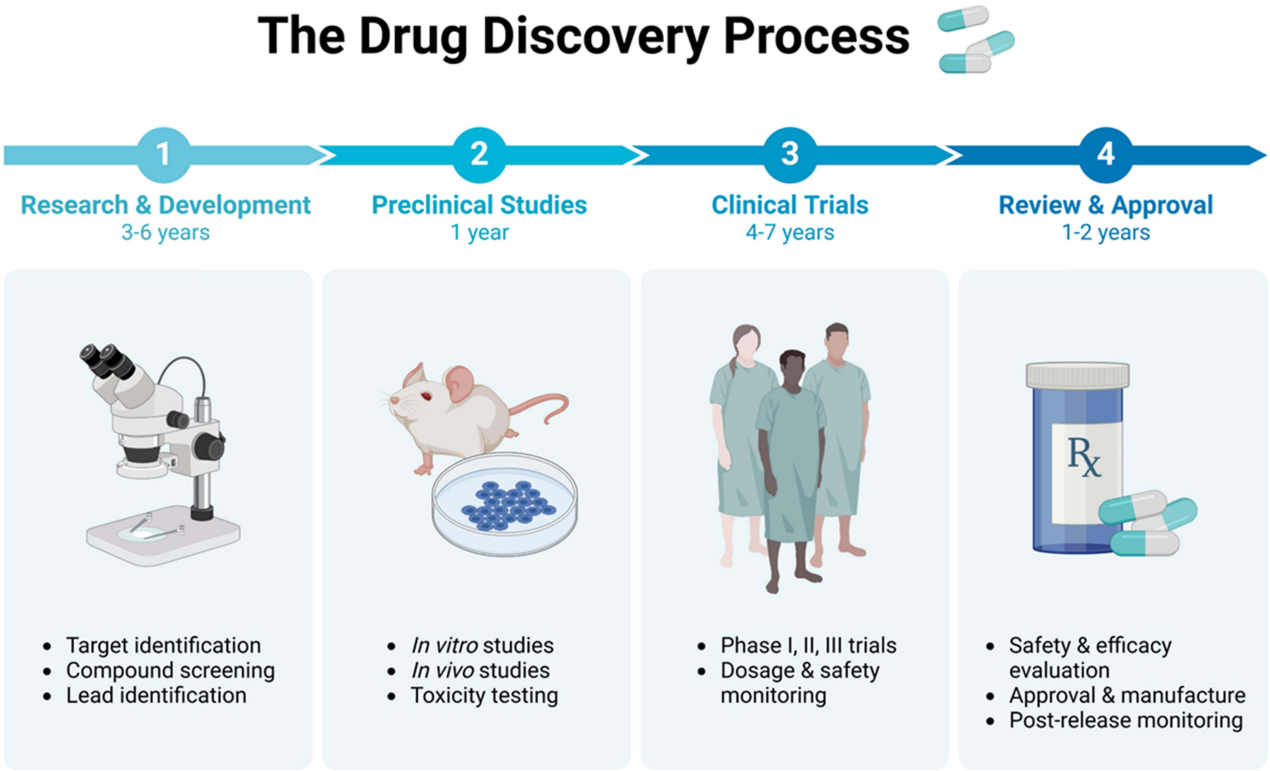

Figure 2 The drug discovery process.
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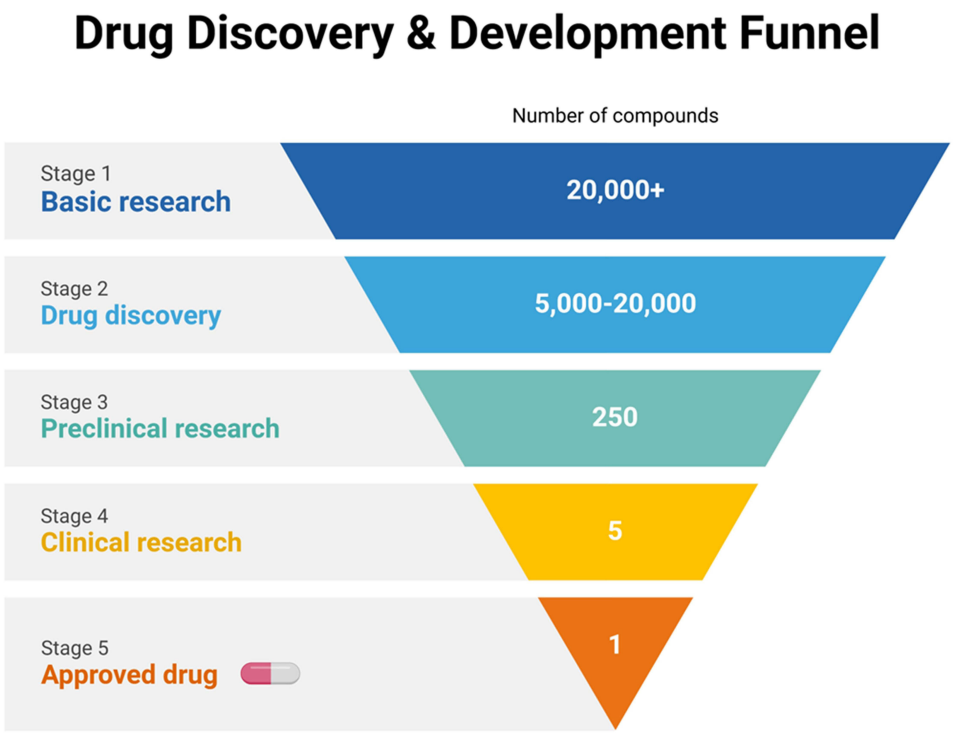

Figure 3 Drug discovery and development funnel.
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AI-Driven Innovations in Oncology

The demand of newer discoveries in the current era is increasing, shading the light about a faster and accurate medication production. Cancer is one of evolving diseases that become a major threat to humanity regarding health and a common challenge facing medical research institutions worldwide.[30] The World Health Organization declared that cancer occupies the first or second rank among the leading reasons for death in 91 out of 172 countries.[31,32] In the beginning, several anticancer agents were isolated from plants, such as taxol, vinblastine, vincristine, derivatives of camptothecin, etoposide, irinotecan and topotecan.[33] An ideal anticancer agent from a plant should have anticancer properties and a defined mechanism of action with minimal toxicity.[34] However, several drawbacks (eg, poor pharmacokinetics, low potency, and remarkable toxicity) hinder the transition of such anticancer agents from bench to clinical trials because of its established poor pharmacokinetics, low potency, and remarkable nephrotoxicity.[35]

In cancer research, AI is expanding because of its huge and different successful applications including the development of new medicines to treat cancer.[36] Numerous of AI researches nowadays have been investigating the widely utilization of incorporating AI to develop newer anticancer medicines by using an association analysis algorithm that identifies cancer and treatment connection (eg, cancer immunotherapy) to select and prioritize cancer-specific drugs.[30] AI with modern data assets accelerates the design and development of safer and more effective anticancer drugs.[37]

The Role of AI in Accelerating Drug Discovery, Enhancing Drug Efficacy and Minimizing Toxicity

Recent research focused on the role of AI in accelerating drug discovery and enhancing cancer treatment, including machine learning and deep learning, that innovating various aspects of oncology, from target validation and drug repositioning to de novo design and clinical trial optimization.[38] These developments enable the rapid identification of new compounds, optimized dosages, and enhanced treatment efficacy with reducing toxicity.[39,40] AI can analyze massive datasets, improve drug response predictions, enhance the accuracy of diagnostic imaging, and facilitate personalized medicine approaches.[41,42] The application of AI nowadays widely varies in different fields. One of which is the medical

field that has showed an improvement and enhancement in the productivity, consistency and accuracy of health professionals.[43,44] Despite challenges such as data quality and model interpretability, AI promises to revolutionize cancer care by accelerating drug development, reducing costs, and improving patient outcomes.[45,46]

As an example of a recent and practical study for the use of AI in cancer therapy discovery in 2025,[47] a study published in Nature Communications that developed a multi model framework for identifying synergistic drug combinations against pancreatic cancer. There are three research institutions (NCATS, MIT, UNC) were built machine learning models based on preliminary experimental data from testing 496 combinations of 32 anticancer drugs using PANC-1 cells. Several algorithms including Random Forest (RF), XGBoost, Deep Natural Network (DNN), and Graph Convolutional Networks (GCN), were used to extract synergistic predictions for 1.6 million possible combinations. The MIT model achieved the highest predictive accuracy with 83% success rate in laboratory trials among the combinations proposed, and 307 synergistic drug combinations were verified as effective. It is worth noting that the compound collection used includes approved drugs and investigational drugs in various stages of clinical trials, which make their manufacturing and clinical application a realistic prospect. So, the study highlighted the potential of machine learning in predicting drug synergies and its practical impact in identifying combinations for treating pancreatic cancer and demonstrates the effectiveness of using multiple machine learning approaches in predicting drug synergies for pancreatic cancer.

Subfields of AI for Developing New Medicines

Machine learning (ML) is a subfield of AI that applies statistical methods with the ability to learn with/without being explicitly programmed. The ML is classified as supervised, unsupervised and reinforcement learning. Supervised learning comprises methods of regression and classification, where the predictive model is developed depending on data coming from input and output sources. Output data from supervised ML includes the diagnosis of diseases under the classification subgroup as well as the prediction of drug efficacy and ADMET (absorption, distribution, metabolism, excretion, and toxicity) under the regression subgroup.[48,49] In unsupervised ML, on country, it comprises methods of clustering and feature-finding by grouping and interpreting data depending on the input data. Outputs from the unsupervised DL attain discovery of disease subtype from clustering and discovery of disease target from feature-finding. However, reinforcement learning is largely driven by decision-making in a certain environment and its execution to maximize its performance. The outputs from the reinforcement ML include a design of de novo drugs under decision-making and experimental designs under execution, which are achieved via modeling and quantum chemistry. While DL showed a greater benefit previously, the increasing amount of database required a growing power and further advancement in this technology. Consequently, deep learning (DL), which is an extra subfield of ML, has emerged with the utilization of artificial neural networks that learn and adapt from the enormous amount of experimental data (Figure 4).[48,50]

In 2025, a study using ML and DL methods to develop drug discovery with some algorithms.[51] This study integrates multi-omics data and AI-driven drug discovery to identify TNFRSF10A/TRAILR1 as a potential therapeutic target in pancreatic ductal adenocarcinoma (PDAC) that proposing an antagonist approach with Temsirolimus, Ergotamine, and capivasertib as potential TRAILR1 modulators. The study provided several significant insights, including identified TNFRSF10A/TRAILR1 as potential therapeutic target in PDAC with high expression in malignant epithelial cells and stromal regions. Additionally, the study proposed an antagonist approach to targeting TNFRSF10A that differs from traditional agonist approaches, as well as, demonstrated the effectiveness of integrating multi-omics data, ML, DL, and molecular dynamics simulations for drug discovery. The authors concluded that their approach showed how combining cutting-edge genomics, system biology, and AI could give us a reasonable insight into most treatment-resistant cancers and suggesting that the study indeed provided valuable insights into treatment PDAC and drug discovery.

AI Versus Conventional Pharmaceutical Approaches in Developing New Medicines

Conventional pharmaceutical methods were relatively successful in discovering new drugs. Unfortunately, the existing drawbacks and limitations of low-grade reliance on trial-and-error experimentation and inaccurately predicting the behavior of newly discovered drugs limit the use of this method.[52,53] On the other hand, AI-incorporated technologies

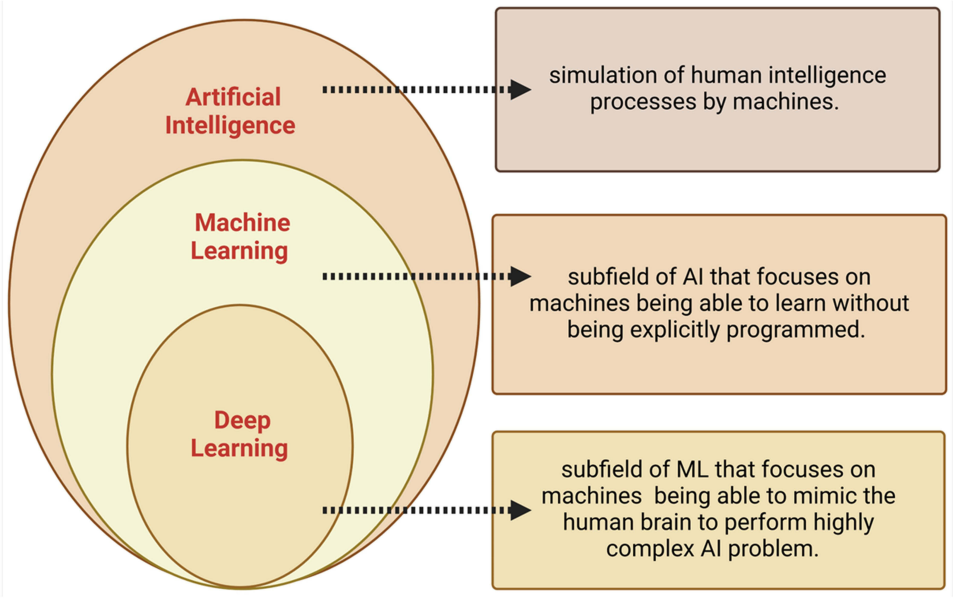

Figure 4 Subfields of AI. (AI vs ML vs DL).
Notes: Created in BioRender. Ghanim, F. (2025) https://BioRender.com/mptkfg2.

have become versatile tools, which are applied in the different stages of drug development, including drug target identification and validation, rational drug design, novel drug designing, drug repurposing, improvement of the R&D efficiency, analysis of biomedicine information and refining the process of decision making.[6,54,55] These potential uses of AI offer better opportunities to counter the uncertainties and inefficiencies arising in conventional drug development methods, minimizing human bias and intervention.[6,54,55] However, recent developments in AI, including the utilization of data augmentation, explainable AI, and the integration of AI with traditional experimental methods, offer promising strategies for overcoming the challenges and limitations of AI in the context of drug discovery.[53] Despite the successful application of AI in developing new drugs, the limitations of AI-based methods, the availability of high-quality data, and addressing ethical concerns are required to be recognized and addressed.[53,56]

Although recruiting the current AI-based approaches in developing new drugs, they will not replace the conventional experimental methods, or dispense with the experience of researchers. Conversely, the role of AI-based approaches will assist in providing predictions relying on the available data, while the validation and interpretation of the results will be still supervised by researchers. Hence, a collaboration between pharmaceutical and AI researchers and a combination of their experience and knowledge will be crucial in creating powerful algorithms and machine-learning models to predict the efficacy of potential drug candidates as well as accelerate and optimize drug discovery.[53,56] Additionally, this integration is beneficial in better identification of new drug targets and improving the effectiveness of the existing drugs toward a better quality of life. In the clinical trials, AI will assist in improving the accuracy and efficiency of the agents since the higher efficiency and accuracy of AI algorithms in analyzing the collected data during clinical trials can result in identifying trends and potential side effects of the candidate drugs as well as improving accessibility and affordability of healthcare.[53]

The design of novel drugs is a fundamental function of AI in drug discovery with specific properties and[57] activities. For instance, a recently trained DL algorithm on a dataset of known drug compounds and their corresponding properties established that AI could rapidly and efficiently propose new drug candidates with desirable solubility and activity.[57] Applying AI in pharmaceutical research improved the prediction of efficacy and toxicity of potential drug molecules, enabling the development of more effective and safer medications as well as accelerating the drug discovery process.[53,58] In medicinal chemistry, a key application of AI is to predict the efficacy and toxicity of candidate drugs. Relying on analyzing large amounts of information, ML algorithms identify trends and patterns unrealized by researchers and achieve this task faster than classical protocols, resulting in proposing new bioactive with minimum adverse reactions

(side effects).[59] For example, a trained DL algorithm, using a dataset of known drug molecules along with their corresponding biological activities, could accurately predict the activity of the new compounds. In addition, recruiting intensive training utilizing databases of known safe and toxic compounds for ML could contribute to preventing toxicities of potential drug molecules[59] Classical protocols of drug discovery, on the other hand, frequently depend on slow and costly laboratory experimentation to evaluate the pharmacodynamics of the candidate drug, while the results often remain uncertain and vulnerable to a high degree of variability.

Applications of AI in Oncological Drug Development

There are wide range of AI applications that can be used in the discovery and development of drugs for treatment oncology as shown in Figure 5 and Table 1.

Computer-Aided Drug Design (CADD)

AI enables computers to participate with humans in drug discovery. Such a task is rational and relatively successful as discussed earlier. This is the era of information and information technologies based on the availability of huge and diverse information content of digitalized datasets, which are used across the whole pipeline of drug discovery, starting by identifying drug target, followed by drug design through using several in silico tools. In the previous decade, the design of drugs was accomplished by computer-aided drug design (CADD), which minimized the risk of later rejection for the lead drug molecules, and the CADD has been still in use for drug design even after introducing high throughput screening (HTS) as a result of its high success rates of hit compounds identification and prioritization of HTS active compounds. Predicting binding site while analyzing medication dynamics to the target are one of the most common applications of CADD with large database. This suggests the critical movement of identifying and evaluating newer anti-tumor agents through this approach.[55]

Antibody Design

Several DL approaches have been developed to study drugs of biological macromolecules with specific pharmacological properties, such as oligonucleotides, monoclonal antibodies, or peptides. In antibody discovery, looking for new antibody sequences by applying AI has become a research hotspot. For example, GANs or VAEs are DL algorithms that are

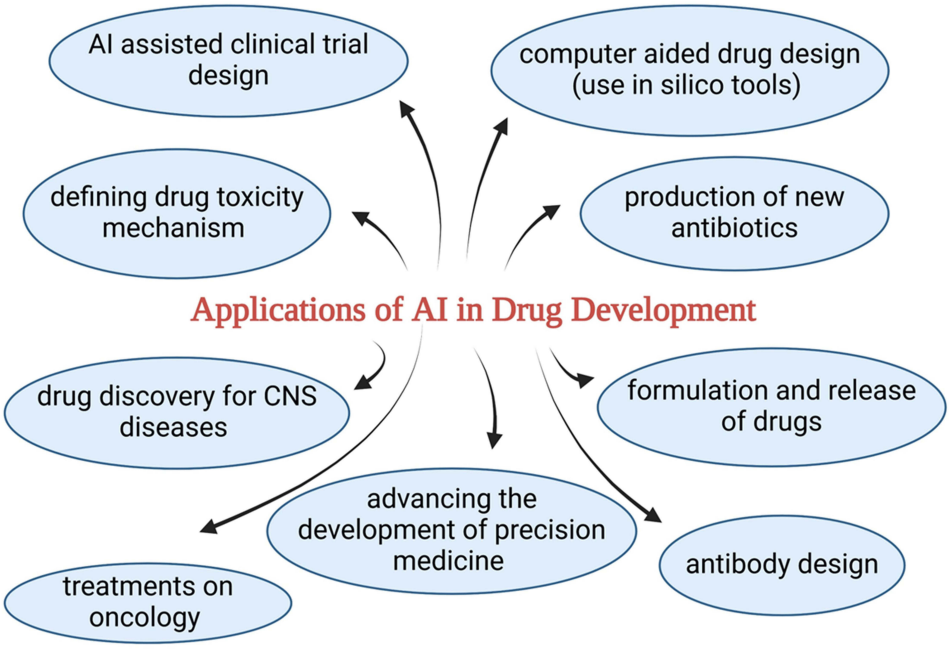

Figure 5 Applications of AI in Drug Development.
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Table 1 AI Models Utilized in the Oncology Application with Techniques Limitations

Algorithm Differences				
AI Algorithm	**Mechanism**	**Application**	**Use in Oncology**	**Cons**
Computer-aided drug design (CADD)[55]	Applies various computational and statistical methods to analyze biochemical entities (Big Data) for target identification and hit hunting. It helps in assessing safety, efficacy, and toxicity for developed drugs.	Identification of binding sites in target proteins, structure-based virtual screening (SBVS) and prediction of pharmacokinetic (ADME) and toxicity (T) properties	Halicin discovery despite being antibiotic, was found to have anticancer activity Facilitate anthraquinone derivative with minimal toxicity and higher efficiency Develop KRAS inhibitor drug targets	1. Accuracy of method needs further validation evaluation. 2. Binding affinity lacks accuracy in the scoring system. 3. CADD Simplify biological system which may produce low-quality of data.
Generative artificial intelligence (GAI)[60]	Use generative models to general new products in the abscess of dataset. This model is trained on the data and use them to improve	Analyze the distribution of the physicochemical algorithm, maximize targeted goal to improve molecular activity, and create newer molecules based on the needed requirements.	Drug discovery for newer anticancer in breast and prostate cancer Analyze pharmacogenomic variation to predict cancer response to therapy.	1. Risk of false positive and inapplicability in the real world suggestions. 2. Fail to generalize the newer produced candidates. 3. Not easily interpreted data (difficult for decision making process). 4. Quality of the generated molecules depends on training data quality.
High-throughput screening (HTS)[61]	A model that tests thousand to million molecules biological activity at cellular, organism, mechanism, and pathway level and provide ranking for their activity.	Improve efficacy and improve success rate of selecting proper therapy for specific cancer type.	Accelerating pipeline drug discovery	1. Lack real world insights due to over-reliance on AI predictions might reduce experimental validation. 2. Biased results according to the reinforce existing data. 3. High false positive results.

learned to explore potential features of antibodies (eg, physicochemical properties and frequency of amino acid positions), providing a new approach for future antibody design and generation.[62]

Treatments in Oncology

AI is used in what is called CyberKnife® treatment in oncology. Moreover, a group of ML algorithms have been recently successfully trained to rank clinically relevant cancer drugs based on the drugs' predicted efficacy in reducing cancer cell growth. One of the successful applications of AI in Oncology is the implication of AI with robotics for radiotherapy.[63] Moreover, AI in Oncology provides a promising application in the area of cancer imaging.[7] However, AI algorithms seem to be promising in solving problems and overcoming obstacles that face discovering and designing new anticancer drugs.[8]

AI-Assisted Clinical Trial Design

One of the most limited steps in the development pipeline of new drugs is the high failure rate of clinical trials so 90% of the drug candidates failed to pass clinical trials. Therefore, several AI-based methods have been developed to assist in optimizing the crucial steps of clinical trials, such as patient recruitment, assignment, and monitoring. For addressing patient selection, AI-based methods are applied to predict the likely treatment response of patients by exploring the association of patients' biomarkers with external indications. Additionally, e-phenotyping can be applied to minimize the heterogeneity of the patient population, aiding the selection of patients through predictive or prognostic enrichment. Moreover, patient monitoring regarding adhering to medication can be controlled by AI because data on accurate adherence to medication reflects the results of clinical trials. AiCure, for example, is a new AI platform that is utilized to measure medication adherence, showing a 25% improvement in adherence to medication in a phase II trial for schizophrenia as compared to conventional therapies. Therefore, AI contributes to reducing adverse reactions and improving the safety of trial protocols by optimizing dosing improving the safety of trial and reducing patient defaults due to safety concerns.[63]

Advancing the Development of Precision Medicine

Adopting various treatment plans for symptoms or diseases of different people is a crucial interest of precision medicine, which is opposite to simplifying or over-simplifying the classification method of diseases using the same treatment plan for all patients. For optimizing precision medicine for each patient, different information is required, including the medical history, results of physical examination, lifestyle, and imaging, results of basic laboratory, functional diagnostics, omics, and immunology. Thus, the collected data are subjected to preprocessing to construct a relevant model reflecting the situation of the patient (Integrating AI in this context has been assessed in various studies. One of which reported that AI connects patient's genomic data, phenotype data, somatic mutation, and proteomics data with the inputted drug response to support further precision medicine. Additionally, many studies suggest that AI can also show the drug response with higher accuracy, sensitivity, and specificity and support knowledge-based production to optimize patient outcomes.[64]

Generative Artificial Intelligence (GAI) in Drug Discovery

One of the latest AI tools that uses DL is generative AI (GAI). The GAI has ability to understand the patterns and intricacy of sets of training data (such as images, audios, and chemical molecules) and subsequently provides predictions based on pattern recognition. This approach, for instance, utilizes to identify de novo molecules and predict drug–target interactions.[65]

When the basic or required molecules are absent from the input chemical library, the prediction-based method is unable to produce new compounds. This is where generative AI (GAI) enters in. Deep learning is used by GAI, a type of AI, to produce original material. After analyzing the patterns and complexity of their training data, in which GAI systems provide fresh data that is either same or better than the user had anticipated. Traditional AI systems taught to analyze data and provide predictions by identifying structures, are not the same as GAI as it relates on the inputted data. The advent of GAI has significantly altered the sector through solving the issue of time-consuming and costly concern to create new

drugs. By automating many of the time-consuming and labor-intensive processes involved in drug development, the GAI technique has the potential to completely revolutionize the industry (Figure 6).

The capacity of GAI models to generate whole new compounds is one of the most alluring aspects of GAI-driven drug discovery. De novo molecular creation is the process of creating new or distinct molecule structures with desired characteristics (Figure 7). Consequently, neural networks that can predict a certain property are frequently included in GAI models. For instance, ReLeaSE, which links a neural network that forecast molecular properties with a deep generative neural network that create novel molecules with the requisite physicochemical and biological qualities, was given in a sample work. The use of ReLeaSE was successfully implemented to produce chemical molecules with specific properties including inhibition activity against Janus protein kinase 2. Thus, the use of GAI can generate chemical libraries that are selective toward a single desired property or multiple properties.[60] Another example was the generated compounds were empirically confirmed to be novel retinoid X receptor (RXR) modulators after[66] training a GAI model

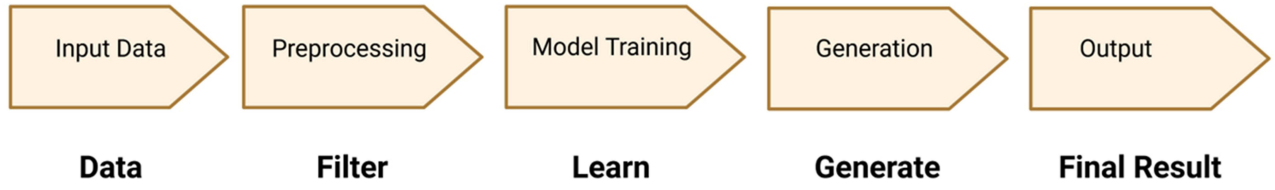

Figure 6 A basic flowchart depicting the functioning of a generative AI model.
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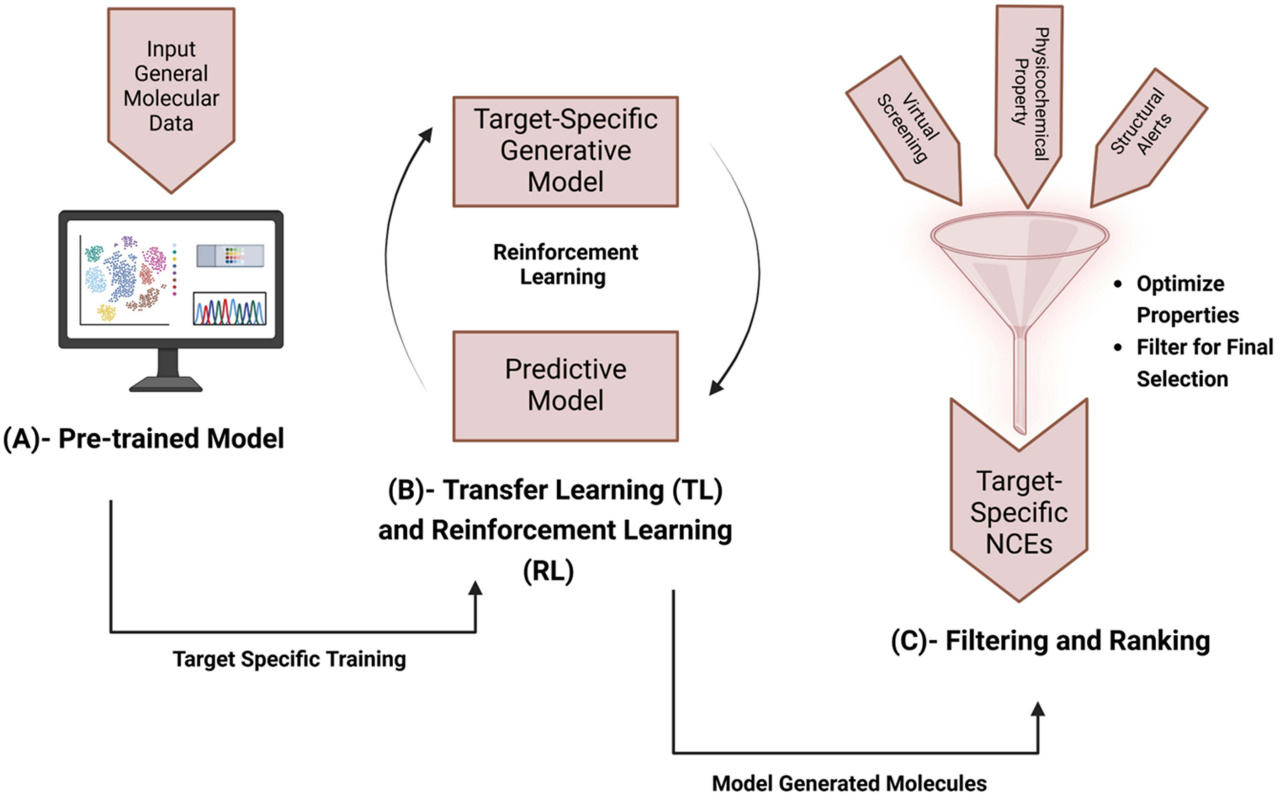

Figure 7 De novo molecular design workflow (**A**) Pre-trained model molecular data. (**B**) TL & RL optimization fine-tune for target optimize properties. (**C**) Filtering and ranking select optimized molecules apply filters and scoring.
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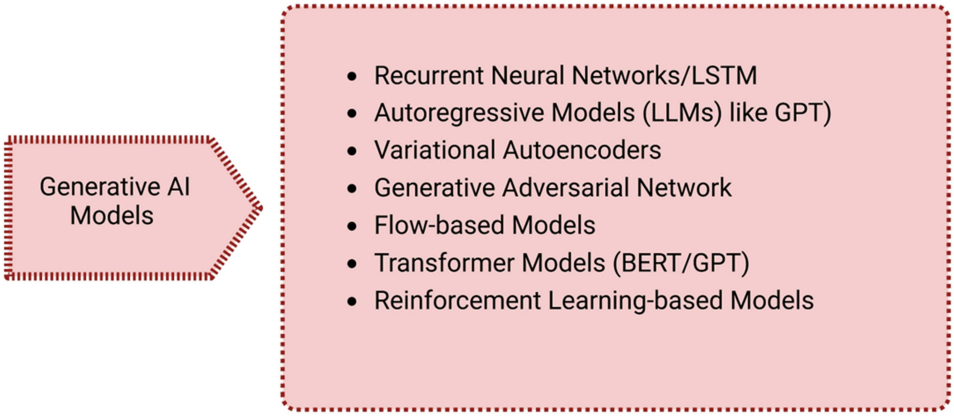

Figure 8 Various GAI models.
Notes: Created in BioRender. Ghanim, F. (2025) https://BioRender.com/wqh6ked.

on natural products to generate de novo ligands. When AI trained system generate four compounds targeting RXR, two of which was found to have resemblance to natural product properties (Figure 8).

In the study for developing a drug for the treatment of lung cancer, an algorithmic framework using deep learning and machine learning to discover novel small-molecule anti-tumor agents for lung cancer,[67] resulting in the derivation of several small-molecule formulas predicted to bind selectively to specific proteins. The study used deep learning for gene expression profile analysis and interaction prediction, Generative Adversarial Neural (GAN) networks for data generation, Lasso linear regression with 5-fold cross-validation for feature selection, and deep learning-based tool for Named Entity Recognition (NER) using BERT algorithm. They identified 37 molecules with potential toxicity for lung cancer cells and five small molecules selected as potential candidates. The algorithmic platform can accelerate the identification and design of anti-tumor compounds that advance targeted cancer therapies. Despite the fact that the study does not evaluate the synthetic potential of the predicted molecules, the researchers deconstructed an initial set of 37 large molecules into smaller active compounds, and this analysis resulted in the addition of 15 additional molecules and led to the selection of five small molecules for further evaluation, this suggested consideration of synthesized potential, even no direct analysis was performed. Therefore, this study used AI in several forms to identify and design new drug use against lung cancer by analyzing genetic data, generating chemical molecules using GANs as GAI, and predicting their effective, all these by using computing study (in silico).

The breakthrough ChatGPT in the recent year grasped the attention through its intelligence system. There has been one recent publication on DrugGPT along the lines of ChatGPT. This study shows AI-driven drug discovery through this approach and further divided GAI into three classes based on how they are used to generate novel compounds:

1. Distribution-learning[68] in which the system creates new molecules to fill the same chemical space as the training set. Metrics such as the Fre'chet ChemNet Distance (FCD), which measures structural and functional similarity, or the Kullback–Leibler[69] (KL) divergence, which is used, for instance, to analyze the distribution of calculated physicochemical features of the molecules, are commonly used to evaluate algorithms for learning distributions based on how well they replicate the characteristics of the training set.
2. Goal-directed generation:[68] that is applied to maximize certain goals, molecules are created in goal-directed generations. To be more precise, scoring functions gradually improve the molecules that are produced. Reinforcement learning (RL) is one way to do this, where a reward is given to the model to encourage it to pursue tactics that have a higher chance of success. Scoring methods frequently employ predicted physicochemical characteristics, expected bioactivity, and resemblance to current active chemicals.[70,71]
3. Conditional generation: By learning a unified semantic space of qualities and structures discovered via exploration, it takes on the problem of creating new molecules that satisfy predetermined requirements. Molecular generation is in the center of conditional generation, which is a goal-directed (using a scoring function), and distribution learning algorithms. The necessary characteristics might serve as a "prompt" to produce possible compounds. By creating

latent representations covering necessary properties like 3D shape,[72] gene-expression signature,[73] protein target,[74] and corresponding molecular structure in an end-to-end manner, for example, via a conditional RNN,[75] these algorithms allow goal-directed generation without the need for scoring function engineering.

Examples of Successful Case Studies of Drug Discovery by AI

AI has been successfully applied to identify novel anticancer compounds by training a DL algorithm on a large dataset of known cancer-related compounds and their corresponding biological activity. Accordingly, high-potential novel anticancer compounds were obtained, showing that IA could discover novel therapeutic candidates.[76] Although developing effective inhibitors of MEK (a suggested target for cancer treatment) is still challenging, the ML algorithm has been described to be successful in identifying novel small-molecule inhibitors of the MEK protein.[77,78]

AI has the ability to identify excepting molecules mechanisms that can treat other diseases such as cancer. One of the examples is Ouabain which was primarily discovered for heart failure patients. Through a High-Throughput Small Molecule Screening AI technique, Ouabain was found among 10,000 molecules to be a candidate synergized with MicroRNA-34 (miR-34) in killing lung cancer cells. miR-34 is a tumor suppressor miRNA that make it target for cancer. Despite the promising results showed by AI in 0.91 sensitivity, there is a need for combination therapy to avoid higher doses of miR-34 which may show toxicity.[79]

Another promising example that enters phase I clinical trials on healthy volunteer was EXS-21546, a highly selective A2A receptor antagonist, which has been co-invented and developed through a collaboration between Exscientia and Evotec SE. EXS-21546, a highly selective drug that is minimally influencing Bain to prevent unwanted event, developed through AI for patients with high adenosine signature solid tumors. Moreover, it is indicated for indicated for the treatment of non-small cell lung cancer, renal cell carcinoma, and advanced malignant solid neoplasms. This advancement supports the process of precision-designed therapeutic candidates[80] (Table 2).

Enhanced Drug Design: Molecular Modeling, Simulations and HTS Screening

AI and Disease Modeling

AI is a revolutionary technology, recapitulating sensing, acting, thinking, and learning that constitutes the four components of human intelligence. Hence, AI can integrate a large amount of structure and non-structured multimodal data to construct dynamic and probabilistic models of the problem.[61] The convergence of AI and biotechnologies offers an opportunity to generate disease models to assist in positioning therapies in known subpopulations of patients to support precision medicine based on therapies that target a definite subgroup of patients. The former convergence can be achieved through performing extensive molecular profiling of the patients with a particular disease to construct disease models. For this purpose, multi-omics technologies are used to represent diseases as endotypes based on pathophysiological mechanisms. In the same line, the data are conventionally generated during the follow-up of huge patient cohorts with a stratification of patients by a combination of supervised and unsupervised learning methods. In the stratification of patients into homogeneous subgroups, the collected molecular profiling data from patients with a particular disease are combined with clinical data (eg, disease severity, disease progression, or response to treatments).[61]

A paper explored how AI techniques applied to model and predict cancer progression, treatment responses, and patient outcomes, by Kumar, 2024.[82] This article is related to AI and disease modeling, specifically in oncology. The main aspects of AI-driven disease modeling discussed and achievement in the article included AI algorithms analyzing high-dimensional genomic data to identify biomarkers that can predict treatment responses and disease progression. ML and DL models are used to classify patients based on their molecular profiles. A notable achievement is the development of adaptive treatment methods using reinforcement learning and neural network-based approaches that allow for real-time therapeutic adjustments based on patient-specific genomic. This article is related to AI and disease modeling focusing on oncology for improving cancer treatment and patient outcomes.

Table 2 Summary of the Successful Case Studies Finding in Utilizing AI Models in the Oncology Field

Applications of AI in Oncology Drugs Discos y and Development					
Study Title	**Year of Publication**	**Objective**	**AI Model**	**Findings**	**Conclusion**
Computational approaches in target identification and drug discovery[55]	2016	To emphasize the necessity of integrating information technologies, chemoinformatics, and human intelligence to enhance data analysis, decision-making, and collaboration in handling large-scale biomedical data.	Computer-aided drug design	Computational methods provided a powerful toolbox for target identification, discovery and optimization of drug candidate molecules. For instance, ligand-based CADD is used effectively in selecting new compounds based in chemical similarity of the active compounds. Additionally, it helped in quantitative structure-activity relationships (QSAR) to describe the correlation between molecules structure and target response. Another application that was gaining ground in the computational drug discovery setting is protechemometrics and polypharmacology modeling. Structural-based CADD has also several applications including studying proteins behavior the rough molecular dynamic stimulation. This can facilitate the other application include docking, pharmacophore modeling, and fragment-based drug discovery.	All the computational methods mentioned in this review, either towards target identification, either towards novel ligand discovery continue to evolve and their synergy is what we envisage that will facilitate cost-effective and reliable outcomes in an era of big data demands.
Artificial Intelligence in Pharmaceutical Sciences[62]	2023	Showing the current application of AI in pharmaceutical sciences while forcing on AI facilitating target and drug discovery	Various models	Many approaches through machine learning (ML) was used to develop medication in the oncological failed. One of which is one-class LR (OCLR) that helps in discovering 13 previously overlooked genes that could be potential targets for LUAD treatment by reducing the cancer's stem-like properties. This is through assisting in calculate different "stemness indices" (mRNAsi, mDNAsi, and EREG-mRNAsi). When it comes to antibodies utilized in oncology, AlphaFold2 which is a deep learning (DL) model helps is understanding protein structure to predict the problem and thus provide suggestions for antibodies. Other models such as structure-based framework called DL for antibodies (DLAB), DeepAb, and DeepH3 were developed to provide extreme precision related to protein structure.	Artificial intelligence widely applies in discovering a developing agent for facilitate clinical trials. Through emerging this intelligence technology, it can solve the complexity of the biological system and correlate it to newer agent.

Evaluating the Effectiveness of Artificial Intelligence in Predicting Adverse Drug Reactions among Cancer Patients[58]	2022	To assess the effectiveness of AI models in predicting ADRs in oncology patients through a systematic review and meta- analysis	Various models (eg: GNB, ANN, XGBoost, ANN-I, RT, KNN, GB)	AI algorithm predict the cytotoxicity of anti-tumor agent through examining the produced bio marker and correlate it with possible toxicities. This through analyzing the sensitivity and specificity of medications' AUC when the patient take anticancer agent to predict the toxicity. It has been seen that a sensitivity values varied from 0.82 to 0.84, demonstrating that the models correctly identified patients who were at risk of ADRs. The effectiveness of AI models is determined by the quality of data used to train them to analyze specific population variables such as the variety of genetic origins, medical histories, or cancer treatment regimens.	AI models can predict ADRs with high sensitivity and specificity. The use of AI in oncology has the potential to revolutionize patient care by combining human clinical decisions with machine-learned insights. However, there is a need for more standardized research in this area, given the variability across studies, to ensure the accuracy and robustness of these predictive tools.
Artificial Intelligence for Clinical Trial Design[81]	2019	Explaining the recent advances in artificial use substantially to the inefficiency of the drug development cycle, in other words intelligence (AI) can be used to reshape key steps of clinical trial design towards the trend that fewer new drugs reach increasing trial success rates.	Neural language	Biomedical reach plays a significant role in understanding cancer. Interestingly, through integrating AI using natural language processing, different subtypes can be identified, predicting gene targets of microRNAs, and discovering new drug-target interactions. Additionally, in clinical trials, AI algorithms show significant identification for skin imaging to detect cancer though digitalized Electronic Records Meaningful Use Programs.	
Effectiveness of Artificial Intelligence for Personalized Medicine in Neoplasms: A Systematic Review[64]	2022	analyze and identify the studies conducted on the application of AI methods in precision or personalized medicine for cancer prediction, diagnosis, and treatment.	DL CNN	AI linked various type of kind, mostly breast and lug cancer, with patient specific factor such as genetic factors, somatic mutation, and phenotype differences. Through determining the differences in genetic makeup, which influence the selection of treatment, AI not only suggest the best agent from the inputted data but also show drug-disease interactions to support knowledge-based production in patient treatment.	Through applying AI-based solutions, this review suggests that AI could improve the treatment and management of cancers and the application of intelligent approaches is recommended in many areas such as in personalized medicine.

AI-Enhanced Drug Design, Selection, and Optimization

In a review article selected, from many examples for AI-enhanced drug design, but not limited, that stated that the field of in silico used to estimate and identify potential of unknown drug-target from large chemical libraries using statistical models known as Virtual Screening (VS) and that ML techniques are applied in VS to enhance predictive performance.[83] This article clearly indicated that VS employs AI techniques for drug design and selection. The VS methods use the physico-chemical and structural properties of compounds with the experimentally verified bio-interaction information to generate predictive models, and these models are utilized to identify new drug candidates for specific targets. This article also mentioned that VS used for drug repurposing and off target effect identification that aim to find new uses for the drugs that already approved, that is a form of AI-enhanced drug optimization. In addition, the article discussed the use of DL algorithms in VS that have showed significantly better for performance drug–target interaction prediction compared to traditional ML methods. Moreover, the VS methods are typically placed just before HTS in drug development pipelines to allow VS to eliminate unlike drug-target that means only potentially active combinations are run through experimental screening procedures, the main purpose of VS is to reduce the cost and time for HTS. This article covered the use of AI and ML approaches in VS for drug discovery and discussed the potential of machine learning -based de novo drug design that is directly related to AI-enhanced drug design and optimization.[83] Although, the VS offers significant advantages in efficiency and potential for improved drug discovery, it still faces challenges related to prediction accuracy, data quality, and computational requirements. Because this field is growing rapidly, that may solve some of these challenges in the future.

The Molecular Modeling and Simulations

Introducing high-performance computing resulted in expanding applications of computers. One of those applications is the utilization of computers as a tool for achieving in silico experiments, including the discovery and design of drugs. Molecular modeling, which is a fundamental tool for discovering drugs, has been developed enormously to enhance the computational power and elaborate biological information of active drugs and compounds. Molecular modeling is commonly applied in the prediction of the target structure, designing novel therapeutic molecules and proposing novel chemical entities. However, throughout the years, recent advancement evolves more which influenced the use of modeling. In pharmacology, for example, molecular modeling used to be a tool for exploring the interaction of drugs with cellular components. However, recent advancements in AI, big data analysis, and molecular simulations provide opportunities to rationalize the interaction of drugs with their pharmacological targets (receptors) such as in silico techniques in some diseases like cancers.[84]

Recently, a promising synergy has been shown between molecular simulations, ML and AI techniques, which will pave the way for revolutionary changes in diagnostics, drug discovery, analysis of medical data, and optimizing clinical trials. Interestingly, it has been found that conventional molecular simulations can be integrated well into AI pipelines, which serve as references and provide data for model training and validation. Molecular modeling provides mechanistic insight into drugs' interaction with their targets (eg, drug–target or drug–membrane interactions), which will provide considerable opportunities to rationalize the design of drug candidates with higher efficacy and minimum side effects better than blindly searching through drug candidates. Computer simulations at the molecular scale will accordingly provide greater understanding of drug behavior and mechanisms of drug toxicity.[85,86]

In an article included molecular modeling, simulations that related to drug discovery in oncology treatment, as example for this specific aspect, in 2021, by Alghamdi et al,[87] this study included molecular modeling as part of a broader investigation into the anticancer potential of Fenugreek seed extracts. The research included molecular docking studies to investigate the interaction between Fenugreek compounds and tubulin that a known target for anticancer drugs. The researchers used Standard Precision (SP) and Extra Precision (XP) scoring functions of GLIDE for docking. The study performed post-docking analysis for the docked poses and calculated binding affinities using Prime MM-GBSA. The researchers also conducted computational predictions of absorption, distribution, metabolism, and elimination (ADME) properties. This article gives us an example of how molecular modeling and simulations can be integrated into a multi-approach to drug discovery in oncology; it is not focused on molecular modeling only, but the study

combined computational methods with experimental techniques to investigate the potential of natural compounds in cancer treatment.

In silico Methods Drug–Target Interaction Modeling

Identifying a pharmacological target, particularly a protein in nature, is the key step in developing a new drug for a certain disease, which can be achieved by a pharmacology network approach either directly by conducting experiments or AI-powered searches. Thus, the identified molecular target can serve as a template for rationalizing the drug design. To accomplish this, the drug discovery pipeline should be adjusted based on the availability of a 3D structure for the target.[88,89.]

Determining the 3D structure of the target protein can be achieved directly through either by crystallography, NMR (Nuclear magnetic resonance), cryo-EM (cryo-electronic microscopy), or indirectly by homology modeling, using a protein of a similar primary sequence. Then, upon knowing the tertiary structure of the pharmacological target, a further investigation for the interaction of the target with the drug candidate can be achieved by using a structure-based method. Otherwise, a ligand-based method is used for identifying drugs with homologies with endogenous ligands if the tertiary structure is unknown. In both situations, virtual screening with other methods is the option for identifying lead drugs.[90]

Using ligand-based methods favorites screening by matching the endogenous pharmacophores of tested compounds with pharmacophores of known drugs, ligands, or drug candidates that are specific for a particular target protein. Instead, the former screening can be achieved by using other QSAR models, which act by estimating the biological activities of the tested compounds in terms of their structural similarities with known ligands. However, AI models frequently excel in the ligand-based method owing to their ability to capture complex, multiparametric, or even hidden structural function relations that can be overlooked by humans. Designing a *de novo* ligand provides an alternative to virtual screening by constructing a ligand able to bind the target with molecular docking or pharmacophore method.[91]

One of the article is more closely related to in silico methods for drug–target interaction modeling is the original study for Alghamdi et al, 2025,[92] the study used computational approaches and web-based tools to predict and analyze the properties, activities, and interactions of metabolites extracted from *Calotropis procera*. The key aspects in this article that supporting in silico drug–target interaction modeling are used the PASS online web server to predict the biological activities of the identified metabolites, including their potential anti-cancer properties, the researchers also employed Swiss Target Prediction to determine potential molecular targets for the bioactive compounds identified in the *C. procera* extract. Moreover, the SwissADME website was used to evaluate the pharmacokinetic characteristics of the identified metabolites, including their adherence to Lipinski's rule of five, solubility, and potential for oral absorption. In addition, the study utilized the ProTox-II website to predict various toxicity endpoints for the identified metabolites, including acute toxicity, hepatotoxicity, cytotoxicity, carcinogenicity, and mutagenicity, as well as, the pred-hERG website was used to assess the potential cardiotoxicity of the metabolites by predicting their likelihood of blocking Herg K+ channels, and the Endocrine Disruptome tool was employed to predict the binding of metabolites to multiple nuclear receptors. The study demonstrated the value of in silico methods in early-stage drug discovery and suggested that further development of these tools could contribute to oncology drug discovery efforts.

HTS and Enhanced Drug

Efficient discovery of drugs is paramount in pharmaceutical research to address unmet medical needs. However, the conventional process of drug discovery is costly and lengthy. However, through introducing high-throughput screening (HTS), drugs revolutionized the pipeline discovery, streamlined the identification of candidates and accelerated the development process.[93] HTS is a process of testing a large number of compounds versus specific biological pathways or targets within a short timeframe,[94] originating between the late 1980s and early 1990s due to the advancement in automation techniques and robotics.[95] Upon combining computational tools with enhanced drug-design strategies, High-Throughput Screening (HTS) can significantly improve efficiency and enhance the success rate of drug development

projects by employing miniaturized and automated platforms for quickly screening compounds, which enables identifying hits with the required pharmacological characteristics.[95]

In the perspective article by Zhou et al, 2025[96] provides several examples that are directly related to HTS in the context of drug discovery and development. The integration of AI and organoids/organs-on-chips (OoCs) has the potential to discover new drugs and development pipeline by enhancing and improve the process. This article mentioned that organoids have employed to model various organs and tissues, including brain, liver, and intestine, they have also used to model a wide range of disease, including genetic disorders, infectious disease, and rare diseases that may be challenging to model. Moreover, several examples of drugs discovered and tested using these approaches are mentioned such as: EXS-21546, an AI-driven drug candidate currently in phase lb/ll trials for patients with solid tumors characterized by high adenosine signatures. INS018_055, an AI-discovered drug that advanced from initial discovery to preclinical testing in 18 months, faster than traditional methods and it is currently in a phase lla study for idiopathic pulmonary fibrosis. In addition, Petosemtamab, TNT005, and HRS-1893, all these drugs have been approved to enter clinical trials based on efficacy and safety data from organoid/OoC models. All these examples demonstrate how AI, organoids, and OoCs are being applied in disease modeling and drug discovery and providing a guide for future applications in this field.[96]

Key Components of HTS

Assay Development

Assay development is the first component of HTS, which is considered the initial step in developing robust and reliable assays (eg, cell-based, biochemical, or biophysical methods) to accurately measure interactions of the screened compounds with targets, involving sometimes a validation of specific readouts for compound potency and target engagement.[94]

Compound Libraries

Compound libraries are the main component of HTS, relying on diverse libraries of compounds with known bioactivities (eg, natural products, synthetic compounds, and small molecules) for screening potential drug candidates. Thus, the utilization of such libraries increased the opportunities to identify hits interacting specifically with the target of interest.[97]

Automation

Automation is a third fundamental component of HTS, which allows a highly speed handling and testing of a large number (thousands or even millions) of compounds by undertaking tasks (eg, compound dispensing, data acquisition and plate handling) to significantly accelerate the screening process.[95]

Data Analysis

A huge amount of data is generated by HTS, necessitating efficient methods of data analysis (eg, statistical, and computational techniques), followed by interpreting the output from screening assays to identify promising hits. Then, integration of data that are generated from multiple assays and a subsequent hit prioritization constitute the crucial steps in HTS workflow.[98]

Advantages and Limitations of HTS

HTS has a variety of advantages, such as throughput, speed, and testing of a wide range of compounds. Additionally, the drug discovery process is expedited since HTS can efficiently identify hits with a potential therapeutic value. Moreover, HTS allows the investigation of biological targets, which enables the exploration of new drug targets either with known or unknown functions. However, inability to perform certain assays due to complex biological systems. Furthermore, synthesizing and acquiring diverse libraries of compounds in HTS is costly as well as HTS may generate false positives and/or negatives due to other experimental variables or test artefacts.[99]

Significance of HTS in Modern Drug Development

In modern drug development, HTS allows for a fast screening of huge compound libraries versus specific biological targets or even disease models. Additionally, the HTS technique benefits from the advancements in data analysis, miniaturization, and automation, enabling the testing of a vast number of compounds in a short timeframe. To rapidly identify active compounds with the required biological properties, HTS can significantly reduce the time as well as cost of identifying lead compounds for optimization and development.[97,98] Furthermore, HTS contributed significantly to enhancing strategies of drug design, resulting in further improvement of the efficiency of drug discovery by employing fragment-based screening computational modeling, virtual screening, structure-based design, and combinatorial chemistry, which assist in optimizing compound libraries and guiding the selection of potential drug candidates. Thus, by integrating these methods with HTS, researchers become able to enhance the identification of selective, potent, and drug-like compounds for further development.[99]

Conclusion

The status of enhancing anti-tumor agents through traditional methods opens the window for research to advance other technologies that reduce expenses and accelerate the drug discovery and development process. Over the past years, AI technology has emerged in the discovery and advancement of medications, offering various models. One such model is CADD, which is utilized to develop potentially interactive molecules with specific biomolecular targets, ensuring their binding and thus improving drug targeting, efficacy, and safety. Another model, GAI, generates new molecules from inputted chemical molecule libraries while also facilitating the activity of these newly generated compounds. Additionally, the HTS screening method integrates the dynamics of the disease or desired effect with large structured or instructed datasets. Through these techniques, AI enhances drug design, targeting, and optimization, ensuring the safe use of newly produced anticancer compounds.

Although AI has a significant impact on this field, it also has several drawbacks that need to be evaluated. One of these is the influence of inputted data, which may play a crucial role in the production of antineoplastic agents. Other considerations include expert evaluation of AI-generated suggestions and results, ethical concerns, and the need for specialized expert support.

In the future, the integration of AI technology in pharmaceutical product development aims to improve the production and advancement of medical agents. Regarding anti-tumor therapies, and given the increasing demand, AI is rapidly accelerating the process of transforming drug candidates into clinical trials. Furthermore, the future of AI in this field highlights its role in predicting anticancer agent toxicity, helping prioritize compounds to minimize drug-related toxicity. Through the continuous development of AI models, the accuracy of drug target identification is steadily improving.

Acknowledgments

The authors would like to thank Marwah I. Bin Abdulqader for her valuable assistance in reviewing and revising the manuscript, restructuring the main sections, preparing tables, and contributing to responses to reviewers.

Author Contributions

All authors made a significant contribution to the work reported, whether that is in the conception, study design, execution, acquisition of data, analysis and interpretation, or in all these areas; took part in drafting, revising or critically reviewing the article; gave final approval of the version to be published; have agreed on the journal to which the article has been submitted; and agree to be accountable for all aspects of the work.

Disclosure

The authors declare that they have no conflicts of interest in this work.

References

1. Yuan H, Ma Q, Ye L, Piao G. The traditional medicine and modern medicine from natural products. *Molecules*. 2016;21(5):559.
2. Hughes JP, Rees S, Kalindjian SB, Philpott KL. Principles of early drug discovery. *Br J Pharmacol*. 2011;162(6):1239–1249.

3. DiMasi JA, Feldman L, Seckler A, Wilson A. Trends in risks associated with new drug development: success rates for investigational drugs. *Clin Pharmacol Ther*. 2010;87(3):272–277. doi:10.1038/clpt.2009.295
4. DiMasi JA, Grabowski HG, Hansen RW. Innovation in the pharmaceutical industry: new estimates of R&D costs. *J Health Econ*. 2016;47:20–33. doi:10.1016/j.jhealeco.2016.01.012
5. Lombardino JG, Lowe JA. The role of the medicinal chemist in drug discovery—then and now. *Nat Rev Drug Discov*. 2004;3(10):853–862. doi:10.1038/nrd1523
6. Mak -K-K, Pichika MR. Artificial intelligence in drug development: present status and future prospects. *Drug Discov Today*. 2019;24(3):773–780. doi:10.1016/j.drudis.2018.11.014
7. Chua IS, Gaziel-Yablowitz M, Korach ZT, et al. Artificial intelligence in oncology: path to implementation. *Cancer Med*. 2021;10(12):4138–4149. doi:10.1002/cam4.3935
8. Karwasra R, Khanna K, Singh S, Ahmad S, Verma S. The incipient role of computational intelligence in oncology: drug designing, discovery, and development. In: *Computational Intelligence in Oncology: Applications in Diagnosis, Prognosis and Therapeutics of Cancers*. Springer; 2022:369–384.
9. Shimizu H, Nakayama KI. Artificial intelligence in oncology. *Cancer Sci*. 2020;111(5):1452–1460. doi:10.1111/cas.14377
10. Patel L, Shukla T, Huang X, Ussery DW, Wang S. Machine learning methods in drug discovery. *Molecules*. 2020;25(22):5277. doi:10.3390/molecules25225277
11. Zhang J, Zhang F, Li H, et al. Recent progress and future potential for metal complexes as anticancer drugs targeting G-quadruplex DNA. *Curr Med Chem* 2012;19(18):2957–2975. doi:10.2174/092986712800672067
12. Klessig DF, Tian M, Choi HW. Multiple targets of salicylic acid and its derivatives in plants and animals. *Front Immunol*. 2016;7:206. doi:10.3389/fimmu.2016.00206
13. Majumder A, Biswal MR, Prakash MK. One drug multiple targets: an approach to predict drug efficacies on bacterial strains differing in membrane composition. *ACS Omega*. 2019;4(3):4977–4983.
14. Peón A, Naulaerts S, Ballester PJ. Predicting the reliability of drug-target interaction predictions with maximum coverage of target space. *Sci Rep*. 2017;7(1):3820.
15. Zeng K-W. Pharmacological targets identification and efficacy analysis of phenylethanoid glycosides from Cistanches Herba based on "target fishing" strategy. *Chin Trad Herbal Drugs*. 2018;2018:173–178.
16. Newman DJ, Cragg GM. Natural products as sources of new drugs from 1981 to 2014. *J Nat Prod*. 2016;79(3):629–661. doi:10.1021/acs.jnatprod.5b01055
17. Lo Y-C, Senese S, Li C-M, et al. Large-scale chemical similarity networks for target profiling of compounds identified in cell-based chemical screens. *PLoS Comput Biol*. 2015;11(3):e1004153.
18. El-Wakil MH, Ashour HM, Saudi MN, Hassan AM, Labouta IM. Target identification, lead optimization and antitumor evaluation of some new 1, 2, 4-triazines as c-Met kinase inhibitors. *Bioorg Chem*. 2017;73:154–169. doi:10.1016/j.bioorg.2017.06.009
19. Li G, Peng X, Guo Y, Gong S, Cao S, Qiu F. Currently available strategies for target identification of bioactive natural products. *Front Chem*. 2021;9:761609.
20. Isgut M, Rao M, Yang C, Subrahmanyam V, Rida PC, Aneja R. Application of combination high-throughput phenotypic screening and target identification methods for the discovery of natural product-based combination drugs. *Med Res Rev*. 2018;38(2):504–524. doi:10.1002/med.21444
21. Yang Y, Adelstein SJ, Kassis AI. Target discovery from data mining approaches. *Drug Discov Today*. 2012;17:S16–S23.
22. Tan S, Chen W, Xiang H, Kong G, Zou L, Wei L. Screening druggable targets and predicting therapeutic drugs for COVID-19 via integrated bioinformatics analysis. *Genes Genomics*. 2021;43:55–67.
23. Lv Y, Ma X, Du Y, Feng J. Understanding patterns of brain metastasis in triple-negative breast cancer and exploring potential therapeutic targets. *Onco Targets Ther*. 2021;2021:589–607.
24. Nakhjavani M, Samarasinghe RM, Shigdar S. Triple-negative breast cancer brain metastasis: an update on druggable targets, current clinical trials, and future treatment options. *Drug Discov Today*. 2022;27(5):1298–1314.
25. Simoes AE, Rodrigues CM, Borralho PM. The MEK5/ERK5 signalling pathway in cancer: a promising novel therapeutic target. *Drug Discov Today*. 2016;21(10):1654–1663. doi:10.1016/j.drudis.2016.06.010
26. Kiriiri GK, Njogu PM, Mwangi AN. Exploring different approaches to improve the success of drug discovery and development projects: a review. *Future J Pharm Sci*. 2020;6(1):1–12.
27. Tran NL, Kim H, Shin C-H, Ko E, Oh SJ. Artificial intelligence-driven new drug discovery targeting serine/threonine kinase 33 for cancer treatment. *Cancer Cell Int*. 2023;23(1):321.
28. Vohora D, Singh G. *Pharmaceutical Medicine and translational Clinical Research*. Vohora D, Singh G, editors.. London, United Kingdom: Academic Press; 2017.
29. Berdigaliyev N, Aljofan M. An overview of drug discovery and development. *Future Med Chem*. 2020;12(10):939–947. doi:10.4155/fmc-2019-0307
30. Chang L, Wu J, Moustafa N, Bashir AK, Yu K. AI-driven synthetic biology for non-small cell lung cancer drug effectiveness-cost analysis in intelligent assisted medical systems. *IEEE J Biomed Health Inform*. 2021;26(10):5055–5066. doi:10.1109/JBHI.2021.3133455
31. Bray F, Ferlay J, Soerjomataram I, Siegel RL, Torre LA, Jemal A. Global cancer statistics 2018: GLOBOCAN estimates of incidence and mortality worldwide for 36 cancers in 185 countries. *CA Cancer J Clin*. 2018;68(6):394–424. doi:10.3322/caac.21492
32. Sung H, Ferlay J, Siegel RL, et al. Global cancer statistics 2020: GLOBOCAN estimates of incidence and mortality worldwide for 36 cancers in 185 countries. *CA Cancer J Clin*. 2021;71(3):209–249.
33. Gali-Muhtasib H, Hmadi R, Kareh M, Tohme R, Darwiche N. Cell death mechanisms of plant-derived anticancer drugs: beyond apoptosis. *Apoptosis*. 2015;20:1531–1562.
34. Amin A, Gali-Muhtasib H, Ocker M, Schneider-Stock R. Overview of major classes of plant-derived anticancer drugs. *Int J Biomed Sci*. 2009;5(1):1. doi:10.59566/IJBS.2009.5001
35. Ren B, Kwah MX-Y, Liu C, et al. Resveratrol for cancer therapy: challenges and future perspectives. *Cancer Lett*. 2021;515:63–72. doi:10.1016/j.canlet.2021.05.001

36. Mynhier M, Nwoku K, Krishna P, Siemers K, Fassett R. Core services that power AI-driven transformation in cancer research and care. *Biochimica et Biophysica Acta*. 2021;1876(1):188535. doi:10.1016/j.bbcan.2021.188535
37. Chin L, Khozin S. A digital highway for data fluidity and data equity in precision medicine. *Biochimica et Biophysica Acta*. 2021;1876(1):188575. doi:10.1016/j.bbcan.2021.188575
38. Yang F, Darsey JA, Ghosh A, Li H-Y, Yang MQ, Wang S. Artificial intelligence and cancer drug development. *Recent Pat Anticancer Drug Discov*. 2022;17(1):2–8. doi:10.2174/1574892816666210728123758
39. Ho D. Artificial intelligence in cancer therapy. *Science*. 2020;367(6481):982–983. doi:10.1126/science.aaz3023
40. Hasselgren C, Oprea TI. Artificial intelligence for drug discovery: are we there yet? *Annu Rev Pharmacol Toxicol*. 2024;64(1):527–550. doi:10.1146/annurev-pharmtox-040323-040828
41. Bhinder B, Gilvary C, Madhukar NS, Elemento O. Artificial intelligence in cancer research and precision medicine. *Cancer Discov*. 2021;11(4):900–915. doi:10.1158/2159-8290.CD-21-0090
42. Pandiyan S, Wang L. A comprehensive review on recent approaches for cancer drug discovery associated with artificial intelligence. *Comput Biol Med*. 2022;150:106140. doi:10.1016/j.compbiomed.2022.106140
43. Agah A. *Medical Applications of Artificial Intelligence*. CRC Press; 2013.
44. Laptev VA, Ershova IV, Feyzrakhmanova DR. Medical applications of artificial intelligence (legal aspects and future prospects). *Laws*. 2021;11(1):3. doi:10.3390/laws11010003
45. Duo L, Liu Y, Ren J, Tang B, Hirst JD. Artificial intelligence for small molecule anticancer drug discovery. *Expert Opin Drug Discov*. 2024;19(8):933–948. doi:10.1080/17460441.2024.2367014
46. Rehman AU, Li M, Wu B, et al. Role of artificial intelligence in revolutionizing drug discovery. *Fundam Res*. 2024;5(3):1273–1287. doi:10.1016/j.fmre.2024.04.021
47. Pourmousa M, Jain S, Barnaeva E, et al. AI-driven discovery of synergistic drug combinations against pancreatic cancer. *Nat Commun*. 2025;16(1):4020. doi:10.1038/s41467-025-56818-6
48. Bishop CM. Model-based machine learning. Philosophical transactions of the royal society a: mathematical. *Phys Eng Sci*. 2013;371(1984):20120222.
49. Chen R, Liu X, Jin S, Lin J, Liu J. Machine learning for drug-target interaction prediction. *Molecules*. 2018;23(9):2208. doi:10.3390/molecules23092208
50. Lee J-G, Jun S, Cho Y-W, et al. Deep learning in medical imaging: general overview. *Korean J Radiol*. 2017;18(4):570–584. doi:10.3348/kjr.2017.18.4.570
51. Sharma S, Singh R, Kant S, Mishra MK. Integrating AI/ML and multi-omics approaches to investigate the role of TNFRSF10A/TRAILR1 and its potential targets in pancreatic cancer. *Comput Biol Med*. 2025;193:110432. doi:10.1016/j.compbiomed.2025.110432
52. Bannigan P, Aldeghi M, Bao Z, Häse F, Aspuru-Guzik A, Allen C. Machine learning directed drug formulation development. *Adv Drug Del Rev*. 2021;175:113806. doi:10.1016/j.addr.2021.05.016
53. Blanco-Gonzalez A, Cabezon A, Seco-Gonzalez A, Conde-Torres D, Antelo-Riveiro P, Pineiro A. The role of AI in drug discovery: challenges, opportunities, and strategies. arXiv 2022. *Pharmaceuticals*. 2023;16(6):891. doi:10.3390/ph16060891
54. Hamet P, Tremblay J. Artificial intelligence in medicine. *Metabolism*. 2017;69:S36–S40.
55. Katsila T, Spyroulias GA, Patrinos GP, Matsoukas M-T. Computational approaches in target identification and drug discovery. *Comput Struct Biotechnol J*. 2016;14:177–184. doi:10.1016/j.csbj.2016.04.004
56. Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Artificial intelligence in drug discovery and development. *Drug Discov Today*. 2021;26(1):80. doi:10.1016/j.drudis.2020.10.010
57. Gómez-Bombarelli R, Wei JN, Duvenaud D, et al. Automatic chemical design using a data-driven continuous representation of molecules. *ACS Cent Sci*. 2018;4(2):268–276. doi:10.1021/acscentsci.7b00572
58. Jang HY, Song J, Kim JH, et al. Machine learning-based quantitative prediction of drug exposure in drug-drug interactions using drug label information. *Npj Digital Med*. 2022;5(1):88. doi:10.1038/s41746-022-00639-0
59. Hansen K, Biegler F, Ramakrishnan R, et al. Machine learning predictions of molecular properties: accurate many-body potentials and nonlocality in chemical space. *J Phys Chem Lett*. 2015;6(12):2326–2331. doi:10.1021/acs.jpclett.5b00831
60. Popova M, Isayev O, Tropsha A. Deep reinforcement learning for de novo drug design. *Sci Adv*. 2018;4(7):eaap7885. doi:10.1126/sciadv.aap7885
61. Moingeon P, Kuenemann M, Guedj M. Artificial intelligence-enhanced drug design and development: toward a computational precision medicine. *Drug Discov Today*. 2022;27(1):215–222. doi:10.1016/j.drudis.2021.09.006
62. Lu M, Yin J, Zhu Q, et al. Artificial intelligence in pharmaceutical sciences. *Engineering*. 2023;27:37–69.
63. Attia YM, Ewida H, Ahmed M. Successful stories of drug repurposing for cancer therapy in hepatocellular carcinoma, To and Cho_drug repurposing in cancer therapy. 2020.
64. Rezayi S, Niakan Kalhori SR, Saeedi S. Effectiveness of artificial intelligence for personalized medicine in neoplasms: a systematic review. *Biomed Res Int*. 2022;2022(1):7842566. doi:10.1155/2022/7842566
65. Gangwal A, Ansari A, Ahmad I, et al. Generative artificial intelligence in drug discovery: basic framework, recent advances, challenges, and opportunities. *Front Pharmacol*. 2024;15:1331062. doi:10.3389/fphar.2024.1331062
66. Merk D, Grisoni F, Friedrich L, Schneider G. Tuning artificial intelligence on the de novo design of natural-product-inspired retinoid X receptor modulators. *Commun Chem*. 2018;1(1):68. doi:10.1038/s42004-018-0068-1
67. Chebanov DK, Misyurin VA, Shubina IZ. An algorithm for drug discovery based on deep learning with an example of developing a drug for the treatment of lung cancer. *Front Bioinform*. 2023;3:1225149. doi:10.3389/fbinf.2023.1225149
68. Brown N, Fiscato M, Segler MH, Vaucher AC. GuacaMol: benchmarking models for de novo molecular design. *J Chem Inf Model*. 2019;59(3):1096–1108. doi:10.1021/acs.jcim.8b00839
69. Preuer K, Renz P, Unterthiner T, Hochreiter S, Klambauer G. Fréchet ChemNet distance: a metric for generative models for molecules in drug discovery. *J Chem Inf Model*. 2018;58(9):1736–1741. doi:10.1021/acs.jcim.8b00234
70. Olivecrona M, Blaschke T, Engkvist O, Chen H. Molecular de-novo design through deep reinforcement learning. *J Cheminform*. 2017;9:1–14. doi:10.1186/s13321-017-0235-x

71. Blaschke T, Arús-Pous J, Chen H, et al. REINVENT 2.0: an AI tool for de novo drug design. *J Chem Inf Model*. 2020;60(12):5918–5922. doi:10.1021/acs.jcim.0c00915
72. Skalic M, Jiménez J, Sabbadin D, De Fabritiis G. Shape-based generative modeling for de novo drug design. *J Chem Inf Model*. 2019;59(3):1205–1214. doi:10.1021/acs.jcim.8b00706
73. Méndez-Lucio O, Baillif B, Clevert D-A, Rouquié D, Wichard J. De novo generation of hit-like molecules from gene expression signatures using artificial intelligence. *Nat Commun*. 2020;11(1):10. doi:10.1038/s41467-019-13807-w
74. Skalic M, Sabbadin D, Sattarov B, Sciabola S, De Fabritiis G. From target to drug: generative modeling for the multimodal structure-based ligand design. *Mol Pharm*. 2019;16(10):4282–4291. doi:10.1021/acs.molpharmaceut.9b00634
75. Kotsias P-C, Arús-Pous J, Chen H, Engkvist O, Tyrchan C, Bjerrum EJ. Direct steering of de novo molecular generation with descriptor conditional recurrent neural networks. *Nature Mach Intell*. 2020;2(5):254–265. doi:10.1038/s42256-020-0174-5
76. Baillif B, Cole J, McCabe P, Bender A. Deep generative models for 3D molecular structure. *Curr Opin Struct Biol*. 2023;80:102566. doi:10.1016/j.sbi.2023.102566
77. Xiao S, Song Y, Wang Z. Nonparametric spatial autoregressive model using deep neural networks. *Spatial Stat*. 2023;57:100766. doi:10.1016/j.spasta.2023.100766
78. Gupta R, Srivastava D, Sahu M, Tiwari S, Ambasta RK, Kumar P. Artificial intelligence to deep learning: machine intelligence approach for drug discovery. *Mol Divers*. 2021;25:1315–1360.
79. Rupaimoole R, Yoon B, Zhang WC, Adams BD, Slack FJ. A high-throughput small molecule screen identifies ouabain as synergistic with miR-34a in killing lung cancer cells. *Iscience*. 2020;23(2):100878. doi:10.1016/j.isci.2020.100878
80. Synapse. EXS-21546: a quick look at its R&D progress and clinical results from the 2023 AACR 2023. Available from: https://synapse.patsnap.com/blog/exs-21546-a-quick-look-at-its-randd-progress-and-clinical-results-from-the-2023-aacr. Accessed June 25, 2025.
81. Harrer S, Shah P, Antony B, Hu J. Artificial intelligence for clinical trial design. *Trends Pharmacol Sci*. 2019;40(8):577–591. doi:10.1016/j.tips.2019.05.005
82. Kumar A, Metta DS. AI-driven precision oncology: predictive biomarker discovery and personalized treatment optimization using genomic data. *Int J Adv Res Publ Rev*. 2024;1(3):21–38. doi:10.55248/gengpi.5.0224.0421
83. Rifaioglu AS, Atas H, Martin MJ, Cetin-Atalay R, Atalay V, Doğan T. Recent applications of deep learning and machine intelligence on in silico drug discovery: methods, tools and databases. *Brief Bioinform*. 2019;20(5):1878–1912. doi:10.1093/bib/bby061
84. Walters WP, Barzilay R. Applications of deep learning in molecule generation and molecular property prediction. *Acc Chem Res*. 2020;54(2):263–270. doi:10.1021/acs.accounts.0c00699
85. Tripathi MK, Ahmad S, Tyagi R, Dahiya V, Yadav MK. Fundamentals of molecular modeling in drug design. In: *Computer Aided Drug Design (CADD): From Ligand-Based Methods to Structure-Based Approaches*. Elsevier; 2022:125–155.
86. Lagoutte-Renosi J, Allemand F, Ramseyer C, Yesylevskyy S, Davani S. Molecular modeling in cardiovascular pharmacology: current state of the art and perspectives. *Drug Discov Today*. 2022;27(4):985–1007. doi:10.1016/j.drudis.2021.11.026
87. Alghamdi SS, Suliman RS, Alsaeed AS, et al. Novel anti-tubulin compounds from Trigonella foenum-graecum seeds; insights into in-vitro and molecular docking studies. *Drug Des Devel Ther*. 2021;Volume 15:4195–4211. doi:10.2147/DDDT.S320793
88. Tabari MAK, Khoshhal H, Tafazoli A, Khandan M, Bagheri A. Applying computer simulations in battling with COVID-19, using pre-analyzed molecular and chemical data to face the pandemic. *Inf Med Unlocked*. 2020;21:100458. doi:10.1016/j.imu.2020.100458
89. Topol EJ. High-performance medicine: the convergence of human and artificial intelligence. *Nat Med*. 2019;25(1):44–56. doi:10.1038/s41591-018-0300-7
90. Lavecchia A, Cerchia C. In silico methods to address polypharmacology: current status, applications and future perspectives. *Drug Discov Today*. 2016;21(2):288–298. doi:10.1016/j.drudis.2015.12.007
91. Lauria A, Bonsignore R, Bartolotta R, Perricone U, Martorana A, Gentile C. Drugs polypharmacology by in silico methods: new opportunities in drug discovery. *Curr Pharm Des*. 2016;22(21):3073–3081. doi:10.2174/1381612822666160224142323
92. Alghamdi SS, Alturki AY, Ali R, et al. Pharmacological profiling of calotropis procera and rhazya stricta: unraveling the antibacterial and anti-cancer potential of chemically active metabolites. *J Cancer*. 2025;16(1):12. doi:10.7150/jca.96848
93. Zhang J-H, Chung TD, Oldenburg KR. A simple statistical parameter for use in evaluation and validation of high throughput screening assays. *J Biomol Screen*. 1999;4(2):67–73. doi:10.1177/108705719900400206
94. Macarron R, Banks MN, Bojanic D, et al. Impact of high-throughput screening in biomedical research. *Nat Rev Drug Discov*. 2011;10(3):188–195. doi:10.1038/nrd3368
95. Hertzberg RP, Pope AJ. High-throughput screening: new technology for the 21st century. *Curr Opin Chem Biol*. 2000;4(4):445–451. doi:10.1016/S1367-5931(00)00110-1
96. Zhou L, Chen S, Liu J. When artificial intelligence (AI) meets organoids and organs-on-chips (OoCs): game-changer for drug discovery and development. 2025.
97. Karczewska N, Pyc M, Żukowski K, Kosman J, Kwiatek D, Kolanowski J. The role and application of high-throughput screening in the search for chemical compounds of therapeutic activity. *Postepy Biochem*. 2024;70(2):230–245. doi:10.18388/pb.2021_528
98. Gubler H. High-throughput screening data analysis. *Nonclinical Statistics for Pharmaceutical and Biotechnology Industries*. 2016:83–139.
99. Paricharak S, Méndez-Lucio O, Chavan Ravindranath A, Bender A, IJzerman AP, van Westen GJ. Data-driven approaches used for compound library design, hit triage and bioactivity modeling in high-throughput screening. *Brief Bioinform*. 2018;19(2):277–285. doi:10.1093/bib/bbw105