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Chapter 10: Artificial intelligence and drug development: Accelerating the discovery of life-saving medications

10.1 Introduction

The discovery of life-saving medications has always been portrayed as the heart of pharmaceuticals. It substantially revolutionized public health outcomes, in relation to the prevention, treatment, and even curing of a vast range of initial terminal ailments. Nevertheless, significant shortcomings have become apparent regarding the traditional methods for developing life-saving medications in an increasingly fast-paced society. The demand for an ever-growing pipeline of innovative pharmaceutical products could often exceed the pace of R&D leading to the delay in granting patient access to them, often even after it had been proved by robust clinical data that the benefits outweigh the risks. Here, the timely access to life-saving medications is declared as one of the main challenges for healthcare and society. There is much hope and belief that both academia and industry players should shift towards unparalleled innovation in order to foster critical advancements in the pharmaceutical sector. The commercial opportunities are considered as vast, in an attempt to address a global market deficit.

In this context, the goal of this report is to investigate and discuss the potential impact of artificial intelligence technologies on pharmaceutical innovation with a focus on their potential to significantly accelerate the discovery of life-saving medications. The essay deliberates on recent and future contributions and analyses AI-driven technologies with broader implications shaping the future landscape of drug development and pharmaceutical delivery. It focuses on the drug discovery phase, discussing how advancements in AI technologies have led to innovation of sophisticated algorithms. These advancements are progressively employed and embedded in the current drug development workflow. The report is structured as follows. It begins with a general overview of modern healthcare challenges, underscoring the necessity by demonstrating the manifest difficulties of the processes in the light of the most significant pathways and targets. Following this interpreted foundation, the essence of the applied AI technologies is deliberated with a more profound and focused analysis on the employed methodologies. The report then extends this discussion on to the integration of different AI technologies to converge on platforms currently utilized in an environment where the old paradigm is being overtaken by the new. It finishes with a contemplation encompassing possible future trends, together with remarks and conclusions ensuring a vastly taken perspective for its importance.

Fig 10.1: Drug Development

10.1.1. Background and Significance

Pharmaceutical research has evolved greatly since the 19th century, progressing from random empiric experimentation to systematic and rational drug discovery and design. The complexity of the drug discovery process is increasing exponentially each year with new emerging technologies, such as CRISPR gene editing and biochips. AI applications encountered in drug development include ML for model complex biology and chemistry, as well as NL methods for extracting pharmacological and biological information . There is a growing need for AI-driven drug design as only 1 in 10 approved drugs survive the clinical trials. Currently, bringing a new drug to the market takes on average 12 to 15 years and costs between 2 to 3 billion dollars. Clinical trials have become increasingly expensive, complex, and slow, often taking over 7 years to conduct. The growth in genetic testing and NGS makes the conducting of clinical trials even more expensive and time-consuming. Particularly in the field of targeted therapies, it is necessary to analyze the patient samples that require the analysis of gigabytes of information. AI empowers the modeling of complex networks and regulatory circuits with multilayered pathways and gene regulation. For example, it is able to model complete signal transduction pathways or the effect of microbial shifts on human metabolism. Mathematical modeling is indispensable for comprehensive understanding. AI has the potential to foster the discovery of more sophisticated pathways, such as the circadian and immune systems. Machine learning, also as a part of AI, is constantly increasing in popularity in the life sciences and is often used to predict cellular metabolism, drug resistance, and metabolic pathways. The assembly of such a network is extremely time-consuming and partly empirical. In this context, AI can contribute by aiding in the identification of relevant players, by learning from the literature. Such generated models can then be used for generating a hypothesis. Recently, methods are being developed that model basic chemical kinetics to model biological systems. On a different note, from the era that morpholin-based drugs were designed, AI-based technology has seen exponential development. Such platforms are not limited to structure prediction, but are capable of determining the sequence and structure activity relationships. This is essential for peptide-based drugs. Determinants of immune cell responsiveness can be inputted into the algorithm and the technology can predict the matching peptides. Early AI methods in drug design were used for generating chemical structures. Additionally, informal networks from big pharma companies and academia were created for sharing experiences. Modeling of enzyme kinetics was carried out to design antibiotics. Early successes of AI in drug design can be considered the structure of the HIV protease inhibitor. Now, however, AI has come a long way. It no longer focuses only on computer chemistry, but has branched into multiple specialties. Moreover, AI platforms are scalable and the ever-growing amount of mammalian and bacterial data ensures their relevancy.

10.2. Overview of Drug Development

Drug development is a complex and lengthy process that is vital to ensure the safety and efficacy of new medications. It involves many phases, from identifying a potential new drug in the laboratory to gaining marketing approval to commercialize it. Several of these phases can be broken down into several stages, each with its attendant difficulties. For instance, the preclinical phase consists of first identifying a lead compound followed by extensive lab testing. Drug development then moves into clinical trials, divided into phases I-III, each more complicated and expensive than the last. After conclusive testing in humans, the new drug must then be officially approved by a federal regulatory body before hitting the market. The average new drug in development takes a decade until it is finally approved and hits the market. Even so, the time spent developing a new drug is invaluable, for it includes all failed attempts as well. This helps to show an annual pattern of successful drugs officially released, which usually occurs in the mid-50s without any revolutionary change.

Hurdles persist after a promising drug enters clinical trials, the phase 3 failure rate is rising and averages around 58%. Therefore, four general alternatives have been proposed to develop new drugs and treatments, but all of them contain serious and limiting restrictions. However, there is a revolutionary alternative that has the potential and the ongoing trial to explore all the drug compound space and far exceed the maximum revenue of any marketed drug. Using these innovative approaches would allow researchers to drastically increase the chances of developing successful and impactful drugs.

Translational impact: Together, this overall understanding of the biomedical, economic, and ethical issues associated with current drug development, as well as the potential efficacy of emerging alternatives, should better inform researchers and professionals in this field how to incorporate AI, taking into account ongoing experimentation to more effectively accelerate the development of life-saving drugs and treatments.

10.2.1. Stages of Drug Development

The development of a new drug is a lengthy, intricate process that involves multiple phases of laboratory testing, animal studies, and clinical trials. There are certain milestones and regulations that must be met before a new drug can be approved by a regulatory authority and made available to the general public. Due to the multifaceted nature of these activities, the use of AI technologies can help to streamline the drug development process. There is also a heavy focus on the optimization of pharmaceutical delivery methods to bring larger and more frequent doses of existing medications to target locations. The development of a new drug is a complex process that can be broadly categorized into two main phases: preclinical and clinical. Preclinical drug development activities involve the optimization of a lead compound, which is a molecule that shows potential therapeutic effects in the lab but has not been tested in humans. This stage consists of several checkpoints, where the chemical and biological properties of the molecule are evaluated. The main evaluation tools used in the preclinical stages are in vitro bioassays, which are performed on cells in a culture dish, and in vivo model systems. The latter are usually animals, such as mice or rats, that are administered the compound and observed for changes in behavior, size, and other factors. Additional methods of evaluation in the preclinical stages are the use of in silico prediction models, which use algorithms to predict the pharmacokinetic and pharmacodynamic properties of the compound. Successful completion of all necessary checkpoints in the preclinical phase allows the progression to clinical trials. Separate regulatory agencies govern each phase of this process. During clinical development, a new drug must undergo four stages of human testing, beginning with a small group of subjects and ending with a large cohort of patients with the target indication. This stage of drug development can be very costly and time-consuming, with the average drug taking over twelve years to bring to market. The method of administration of the drug is also developed in the clinic. Once the necessary clinical trials have been performed, a new drug application (NDA) can be submitted to regulatory agencies for consideration. Approval of the NDA allows for the market availability of the new drug. Despite the long and rigorous pathway to drug commercialization it is a critically important mission. The high attrition rate in bringing new medications to market is both costly to the pharmaceutical companies and means that there remains a high need for medications that do not yet exist (Singireddy, J., 2022; Hara Krishna Reddy Koppolu et al., 2023; Paleti et al., 2024).

10.2.2. Challenges in Traditional Drug Development

The existing paradigm of drug development is riddled with numerous challenges in view of an inherently costly process which takes years to complete and is characterized by high rates of failure. The pharmaceutical industry operates on a business principle centered around 1) discovering a new molecule; 2) characterizing that molecule, i.e., understanding how it interacts with the human body; 3) developing it into a new drug; and 4) seeing it through regulatory approval. Each of these steps encompasses many intricacies and complexities that render the task a daunting one. The clinical development of a candidate drug is intended to ascertain its overall risk/benefit profile in a patient population, which ideally would result in its being approved as a therapy for that particular indication, in which it provides novel benefits compared to current alternatives. However, as it currently stands, the entire process of conventional drug development is far from optimized and relies to a large extent upon trial and error. Drug development is an expensive and risky enterprise. To develop a new chemical entity, pharmaceutical companies must employ a broad platform of scientific knowledge and technical skills. It is a long journey from basic research through drug development, considering that R&D takes 7 or more years to discover and develop drugs. Overall, the process of developing and marketing a new drug demands an average investment of $2.6 billion and nearly 20 years until result achievement. On average, 12% of drugs that pass the first stage of testing on animals can move into clinical trials in humans. This means that drug companies are at risk of losing 88% of financial investment in the laboratory phase. According to the FDA, 95% of new drugs which are tested in a clinical trial fail to reach the market or aren't therapeutically valid. Despite the enormous amount of money and time expended, only 2% of drugs that reach the phase of testing in humans are approved.

10.3. Artificial Intelligence: An Overview

The applications of Artificial Intelligence (AI) remain a pivotal means by which various industries are continuously transformed, re-imagined, and re-structured according to technological development. Healthcare is no stranger to such a profound change. This particular sector has significantly adopted AI-driven technology, bringing with it state-of-the-art tools as an assistant to increase diagnostic accuracy, improve treatment options, optimize the workflow, and support decision-making processes at large. The algorithm's ability to understand and quickly analyze vast data sets has supported the revolution and the transformation of processes – from drug development to the detection of particular health issues – that have long been deemed unrealistic or significantly more difficult to achieve (Singireddy, S., 2023; Singireddy et al., 2024).

The term Artificial Intelligence (AI) can be understood as the simulation of complex, intelligent behavior that can be associated with the human mind. AI technology is therefore used to formulate the ability of creatures to learn, adjust, and turn appropriate actions. This particular area crosses the limits of both artificial psychology and finding automatic information solutions for highly complex problems. Machine learning and deep learning are two examples out of many that give a broader understanding of how to realize artificial intelligence. Frequently, machine learning allows computers to isolate models from data and deal with fresh information in a discovery-based manner. This is often done by allowing machines to optimize specific functionality using real stimulus data examples. Deep learning, a rebrand or transitional neural networking advance, uses many layers for these capabilities.

Fig 10.2: Artificial Intelligence in Drug Discovery

10.3.1. Definition and Types of AI

Artificial Intelligence (AI) is a wide range of technologies that enable machines to exhibit human-like intelligence in performing cognitive functions and tasks previously only doable by people, such as learning and problem-solving. The technologies that achieve AI include computer vision, natural language processing, speech recognition, and machine learning. There are two types of AI; Narrow (or Weak) AI, which is designed and trained for a particular task, and General (or Strong) AI, which is similar to human cognitive abilities and can learn, understand, and apply knowledge. Today's AI technologies are classified as either Narrow or General AI, with the majority of AI today being Narrow AI, the simplest form of AI implementation that only targets one task. The most well-known methods of Narrow AI implementation are machine learning and deep learning. Machine learning and its deep learning subset have shown remarkable capabilities in data analysis and the creation of predictive models. This is due to the algorithms' strength in examining and finding patterns in large datasets, including semi-structured and unstructured data like text or time-series. Machine learning models come in a variety of forms based on functionality, such as regression analysis, decision tree, or random forest categorization. Depending on the challenge one seeks to address, distinct models can be trained to perform unique tasks and produce specific kinds of solutions.

10.3.2. Historical Context of AI in Healthcare

This subsection explores the historical context of AI's application in healthcare. It starts with an early manifestation of AI research, when AI was presented as a research challenge for medicine and healthcare. The reading is used to illustrate the longstanding promises, predictions, and perceptions that arrived with AI in medicine back in the 1970s when AI technologies were first being introduced to the medical community and where AI was seen to be having a hard time. In the following it is shown that these promises carry on into the 2010s, suggesting that the current wave of enthusiasm for AI was almost fated to meet another wave of skepticism from the medical community.

Efforts to match computers with diagnostic medical reasoning date back to at least 1972 when a collection of papers on the subject was produced as part of a symposium. Printed out the papers from that volume are about 1.5 inches thick and include demographics on a quarter of a million people and a summary written in green ink. Those papers anticipate, if not AI per se, at least data conquest and an expanding role for computing in health care. A few years later, clinical decision support systems were introduced in Ph.D. and M.D./M.S. I work at Stanford. A bit more recently, in February 2013, it was asked to allocate funds towards a project; the point of the proposed endeavor is to increase understanding of brain function and illustrate the need for computers that work with vast amounts of health data.

10.4. Applications of AI in Drug Discovery

In an endeavor to expedite the discovery of medications, some pharmaceutical researchers worldwide have partnered with organizations specialized in artificial intelligence (AI) and machine learning. As a result, the applications of such technologies generate discussions about their usefulness in the field, from target identification and compound discovery to patient-meta research or drug coverage strategies. Some of the nuances that underline the fruitful marriage of biopharmaceutic research and AI technologies will thus be initially overviewed. The nascent integration of AI technologies in a formerly innovation-backward and excessively trailing biopharmaceutical sector may be of interest to scholars venturing in the realm. Due to the aging of the global population and the rise of resistance to medication, there is an escalating demand for the discovery of new pharmaceuticals. Thus, biopharmaceutical research seeks to leverage AI technologies that show grounds for elevating the efficiency and accuracy of each stage of drug discovery.

Near the outset of the talk, an overview of revolutionary approaches to deliver drugs in pharmaceuticals over AI technologies can be discerned. AI algorithms will likely hasten the discovery of compounds alongside the improvement of decision-making. Biopharmaceutical research typically requires a wealth of biomedical data, including concords of gene expression, metabolites or proteins. AI-designated algorithms will swiftly unearth insights and patterns, nearly impossible for individuals processing vast volumes of data. Given the transformative potential of AI, there are mounting discussions over his ability and perquisites for conducting biopharmaceutical research. However, the absence of concrete examples is the deterrent to considering the discourse in depth. Thus, it appears judicious to offer two real-world case studies of AI technologies applied in biopharmaceutical research. They could provide concrete proofs of the efficacy of AI and also spark an interest in the audience. The three latter parts of the talk will thus center on the case studies and discuss how the integration of AI technologies into separate stages of drug discovery abolishes profound alterations in current practices. Such alterations could markedly reduce the costs and duration of each stage. Moreover, the slated response will also elucidate the implications of this nascent relationship for transforming traditional biopharmaceutical research.

10.4.1. Target Identification

In drug discovery, a new compound has to be developed as a new drug to fit a specific target. As the first step in drug discovery, target identification is a significant strategy to identify the interaction with a compound-targets for the biological activities information. AI technologies have been developed to analyze biological data for target identification (TI), and this would be introduced for the critical role. The additional approach for successful connection at the gene level by integrating data on siRNA and cDNA, or data at the genome and cDNA (especially on SNPs) is considered. The experimental design approach is able to give an insight into the expected results for an updating knowledge based on the observed data. It is possible to compute an individualized probability of success for a study to detect a target effect of a substantial size. The priorities are to allow the investigator, on the basis of available data, to determine the level of evidence required, and to perform a rigorous analysis of the plausibility and detectability curves by incorporating popular statistical designs.

With the successful completion of the Human Genome Project and rapid advancement of proteomics, there is a large amount of biological data such as genomics and proteomics, and clinical information about biological function, and phenotype. New methodologies are needed to investigate biological mechanisms and paths regulated by entire biological systems as well as drug mechanisms of action simultaneously, which multi-dimensionally analyze and identify data. A new approach is being applied to the drug discovery process using the human physiome, or a “virtual human”. The former approach promises to significantly reduce the amount of experimental measurements required for constructing accurate models of human cells or organs by integrating both prior physiological knowledge and available experimental data within a bioinformatics/Mechatronics framework. The techniques accelerate the breeding of model species, in developing a viable and innovative new paradigm in human drug discovery that promises to lower costs and improve cross-species translation rates. A physiome-based approach to drug discovery is anticipated to offer a comprehensive and holistic understanding of drug function that is not possible using current approaches that divide the human body into distinct disciplines.

10.4.2. Lead Compound Discovery

The process of discovering an effective drug involves a pilgrimage through a pipeline of research stages, starting from an initial idea and culminating with an approved product delivered to market. This sojourn navigates the long and treacherous pathways of testing chemical and biological properties at diverse preclinical stages, such as assays for drug-target interactions or toxicological side-effects. Development produces a feasible candidate translated to human trials in clinical phases I-III, underpinned by progressively larger clinical trials culminating in regulatory requests for market authorization. This translation to the human context is so time consuming and costly that despite its scientific endeavor and innovation, it has become increasingly inefficient in bringing novel therapies to market. These glooming statistics are some of the main driving forces leading to a momentum that might change the way drug discovery has been conducted for the last decades, coupling it with advances in computer science in what has been termed as Artificial Intelligence (AI).

Recent AI algorithms are revolutionizing the analysis of extraordinarily diverse biological data to predict how small-molecules interact with intricate biological systems. When tailored to model drug-host interactions, these algorithms do foster the emergence of a new research pipeline with transformative potential for pharmaceutical and biotech industries. Besides the possibility of modeling known drug-host interaction conserving the chemical generality of the drug of interest, these models entail great promise for redesigning the chemistry of drugs capable of maximizing a predetermined on-target effect while reducing off-target effects. Several studies have demonstrated these concepts in antibiotic resistance, directly validating the effectiveness of this AI-based approach. These computational techniques can be applied to investigate the drug ability of target proteins or genomes without available proteins, allowing the identification of a new antimicrobial drug in Mycoplasma genitalium. Time and financial worth lead to minimizing experimental testing, and hence the ancillary resources required to align expectations. Online implementation of machine learning algorithms further enables constant learning feedback from new compounds entered in the libraries. Thus, the quality and abundance of learned compounds predict the improvement of future compounds iteratively fine-tuning the approach.

10.5. Machine Learning Techniques in Drug Development

In the life sciences sector, the unpredictable nature of drug interactions, coupled with the significant time and financial requirements, inspired the integration of Artificial Intelligence (AI) to facilitate medication development. AI involves the creation of intelligent systems that think, learn, and act in a way that simulates human intelligence. It encompasses various methods, machine learning (ML) standing out as the most popular. That is a type of artificial intelligence that provides computers with the ability to learn without being explicitly programmed.

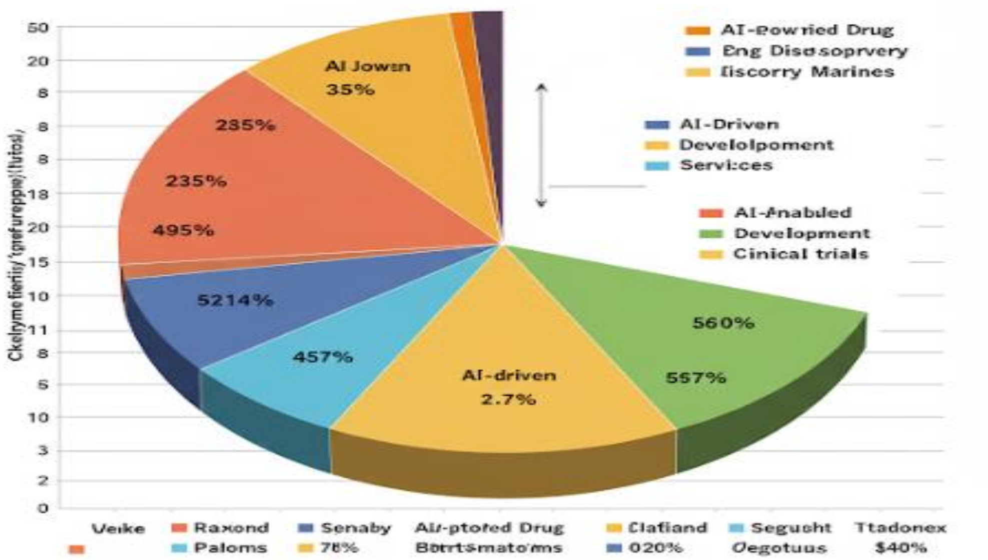

Fig : Artificial Intelligence (AI) in Drug Discovery Market

It has emerged as the tool for data analysis, involving the development of new algorithms capable of interpreting vast datasets. Ranging from building models to predict and customize patient-drug responses to decreasing the time spent on combining symmetric structures, ML tools are transforming the medical and pharmaceutical landscapes. Numerous systems have been developed to identify compounds with the potential of turning into lead drugs, segregate large datasets into classes associated with their pharmaceutical activities or study the large scale-off target interactions between small-molecule drugs and protein targets. Such rapid and scalable work stands to be vital for the advancement of drug development, a field reliant on understandings of biological systems and chemical compounds that exceed the scope of human capability since the distinct timescale thereof is too extensive. Machine learning drastically expedites the time and efficacy needed to analyze complex processes while delivering results amenable to human interpretation. Several approaches have been explored for the development and evaluation of pharmacokinetic parameters as well as the discovery of influential properties defining structure-toxicity relationships. Assorted tools have applied the machine learning system used for the design and interpretation of drug metabolism studies with long-term use, meanwhile others have engineered a platform used for predicting multidimensional aspects of clinical outcomes in trials of neurological medications. Many more systems have been indicated in the supplementary file, covering an array of applications within the pharmaceutical field. With the proper choice of algorithms and hyperparameters and attention to preprocessing, machine learning affords tackling a broad sweep of medical and pharmacological research needs efficiently and effectively.

10.5.1. Supervised Learning

This section is dedicated to machine learning approaches in drug development. As a subfield of artificial intelligence, machine learning represents a set of algorithms and statistical models which allow computers to perform a specific task without using explicit instructions. Labeled datasets lie at the core of machine learning training, facilitating the execution of algorithms on predictive tasks. As a result, algorithms learn underlying patterns of the data, making them capable of making predictions on novel, unlabeled datasets. Training data must consist of input features, or predictors, and the result of interest, that is, the outcome or the dependent variable. Supervised learning, as the name suggests, refers to the process where the outcome is known and the purpose is to find a relationship between input features with the given outcome. Drug development heavily relies on machine learning methods like supervised learning to identify the relationship between specific characteristics of the drug, such as chemical structure or biological activity, and the outcomes of interest, most commonly, drug efficacy. Supervised learning is widely implemented in pharmaceutical research due to its potential in numerous applications alongside drug discovery and design, such as toxicity prediction, stratifying patients based on genetic profiles, and identifying the sub-population from which an individual would most benefit from a particular medicine.

The principal challenge in the context of machine learning models is centered on their accuracy and the trade-off between overfitting and generalizing. As models become increasingly complex, the risk of overfitting grows, thus making them inadequate in generating accurate predictions on novel, unseen datasets. To avoid such issues, models should either generalize or display only a slight drop in performance. Different strategies are aimed at enhancing the generalization capabilities of the supervised learning algorithms. The k-fold cross-validation method is the most common technique, which distributes the given data into k subsets, termed folds. As the process iterates, each fold is held out as a validation set, while the others are used for training the model. Additionally, multiple, independent training and testing datasets generated through the process of resampling are crucial to obtain more reliable estimates of the model's performance. An illustration of case studies of successful applications in drug research fueled by supervised learning, accentuating the vast improvements in the drug design and development process, sheds further light on these approaches and the merits it has to offer.

10.5.2. Unsupervised Learning

Unsupervised learning (5.2) is a machine learning technique that is distinctive from supervised learning. While supervised learning (classification and regression) analyzes a labeled dataset that contains input-output pairs for the model to learn from, unsupervised learning algorithms analyze unlabeled data to understand its patterns and hidden structures. One of the ways in which unsupervised learning can be carried out on a dataset is through clustering techniques, where algorithms organize the data into groups characterized by its own similarities. Another broad category of unsupervised learning algorithms falls into dimensionality reduction approaches which concentrate on capturing the main characteristics of the input dataset in fewer dimensions. Unsupervised learning has the potential to reveal significant insights from intricate datasets, providing potential insights for a new target identification or therapeutic pathway. Given that the unsupervised model learns about the world by itself, extra care usually needs to be taken in regard to its interpretability and validation. However, unsupervised learning can nevertheless be a powerful supplement to the supervised techniques when validation and interpretability are precisely scrutinized. Real-world examples will illustrate some of the many ways in which unsupervised learning can be productively employed in pharmaceutical research and how some of its challenges can be addressed. Through this analysis, it will be demonstrated that a diverse repertoire of machine learning approaches, not limited to the supervised techniques, can bolster drug development initiatives. It has been more than two years since COVID-19 began its relentless global spread, and infection rates have never been higher. While vaccines have played an essential role in the effort to combat the disease since their inception, the way these breakthroughs have been achieved has evolved over time. Companies at the vanguard of this effort have begun to use cutting-edge bioinformatics to develop these significant advances, specifically the identification of vaccine targets for the current pandemic. This will focus on the application of advanced bioinformatics and pharma that enables a more precise approach to the identification of potential drug and vaccine candidates, which involves specific focus on the role of the current pandemic and similar diseases. It contributes to laying the groundwork for the development of unprecedented point-of-care treatments. At the same time, it contributes to setting the rules for the broader application of advanced bioinformatics in the next deadly pandemic and other drug development endeavors.

10.6. Conclusion

In conclusion, current research has highlighted the need to prioritize interdisciplinary collaboration in relation to the growing importance of artificial intelligence (AI) in the development of pharmaceuticals. This expanding area of research has increasingly enabled new achievements and advancements in a variety of applications, particularly in the field of target identification and lead compound discovery. Recent research has utilized and further developed a variety of techniques for a more efficient integration of AI methods. Such applications have already demonstrated their potential to accelerate the discovery of new drugs. The use of neural networks, deep learning models, and affinity learning methods provides a cost-effective alternative to the high-throughput screening of compounds. Moreover, insights obtained from comprehensive bioinformatic databases can expand the number of targets that are considered for drug development. Computational models are capable of simultaneously responding to issues of interest in various fields. Despite their wide scope of activity, they deliver reliable results that extend current knowledge of drug-target interactions. It should be anticipated that the possible applications of AI techniques are by no means limited to those developed so far.

There is no doubt that this fast-growing field will further revolutionize the foundations of the pharmaceutical and biotechnological landscape, not just in terms of the increasing number of drug compounds being developed or discovered, but also, and perhaps foremost, by enhancing the method of their discovery. With the development of novel technologies and the ongoing exploration of innovative methodologies, AI applications in drug development are expected to become an even more major issue in the foreseeable future.

10.6.1. Future Trends

With the development of artificial intelligence (AI) technologies, the project drug development efficiency regulation will have greater transformation. It is expected that machine learning (ML)-, data Mining-, and other types of AI will naturally evolve and combine for more sophisticated platforms. The improvement in AI technologies will also boost modern quantitative approaches for drug discovery and reinforcements. The analyzed data is expected to scale to 70% due to the development of genomics, biotechnology, and other acute technologies, which will allow for a more understanding of the diseases and the effects of therapies. This, in turn, paves the way for the increased advancement of personalized medicine. Ethical standards, regulations, and the views of the population may not be the current development of science and innovations. Therefore, the regulation system is required to be more flexible in evaluating the rapidly changing technological development in order to philosophize its safe and efficient integration into the clinical setting. It is also emphasized that there is a need to enhance cooperation between a rigid company, academic researchers, and relevant regulatory authorities to unlock the potential of accelerating drug discovery life-saving medication compounds. Market competition and financial interest lead to a low degree of sharing research data. However, if computational power and data availability improve, drug discovery will significantly speed up within AI, which provides 10,000 compounds to manage researchers with drug discovery libraries. In many cases, it is difficult to calculate the metric similarities of compounds belonging to different sets. Thus, it is suggested that AI-powered platforms be available as library guest interfaces, which will enable the analysis of all compounds of interest. While this development will drive scientific progress and new business models and will significantly speed up drug discovery. Any drug interaction with the human body may be side effects, which is why there is a safe need for very legislation and regulation enforcement and monitoring.

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