The role of artificial intelligence in drug discovery: Accelerating the development of new medicines

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Abstract---Background _ Drug research and development (R&D) is a complex and lengthy process characterized by high costs, risks, and regulatory hurdles. It involves a multidisciplinary team of scientists, clinicians, and regulatory experts working collaboratively to bring innovative therapies to market. The process typically encompasses several stages, including target identification, drug discovery, preclinical and clinical testing, regulatory approval, and post-market surveillance. Aim of Work – This review aims to provide an overview of the drug development process, highlighting the critical role of technology and management in optimizing efficiency, reducing costs, and accelerating time-to-market. Methods – A comprehensive review of relevant literature was conducted to explore the various stages of drug development, challenges faced by the pharmaceutical industry, and the emerging role of technology in addressing these challenges. Results – Drug development is a high-stakes endeavor characterized by significant investment and uncertainty. Advancements in technology have transformed the drug discovery process, enabling researchers to identify potential drug targets more efficiently and
screen vast chemical libraries rapidly. The integration of artificial intelligence and machine learning has accelerated drug design and optimization. Clinical trials, a crucial phase of drug development, have also benefited from technological advancements. Electronic data capture (EDC) systems and patient-centric technologies have streamlined data collection and management. Real-world evidence (RWE) generated from electronic health records (EHRs) has emerged as a valuable tool for post-market surveillance and drug safety monitoring. Effective drug development requires robust project management and efficient resource allocation. The application of advanced management techniques, such as project management software and data analytics, can optimize decision-making and mitigate risks. Conclusion – The pharmaceutical industry is undergoing a transformative phase driven by technological advancements. By leveraging innovative tools and strategies, the drug development process can be streamlined, costs reduced, and patient outcomes improved. Continued investment in research and development is essential to address unmet medical needs and deliver life-saving therapies.

**Keywords**--- Drug Development, Pharmaceutical Industry, Clinical Trials, Technology, Artificial Intelligence, Drug Discovery, Drug Administration, Drug Management.

**Introduction**

Currently, the process of drug research and development (R&D) is becoming increasingly challenging due to the increased difficulty in obtaining potential leading compounds and the associated costs and risks associated with bringing a drug to market [1]. Market-oriented drug research and development necessitates not only the development of more innovative ideas from scientists, but also the integration of resources, multidisciplinary collaboration, and both on-site and remote collaboration [2]. The European Medicines Agency (EMA) announced on July 18, 2018, that a carcinogenic impurity was discovered in the blood and heart drug valsartan, which was supplied by Zhejiang Huahai Pharmaceuticals in China (https://getzpharma.com/articles/__valsartan). The European Medicines Agency (EMA) and the Food and Drug Administration (FDA) of the United States recalled the raw material medicine Valsartan from the market and promptly prohibited its importation [3,4]. This case is a clear indication that modern administration has a substantial impact on drug research and development and drug marketing. Modern administration necessitates the expeditious integration of numerous resources. We will strive to enhance the benefit of patients by effectively enhancing the development of innovative drugs and the monitoring of drugs in the market by increasing efficiency and optimizing the use of modern science and technology and innovative ideas [5,6]. This article will delve into the specifics and the extent to which management science is involved in each stage of the drug discovery and marketing process.
The comprehensive procedure of medication research and development and drug marketing

The process of drug discovery is lengthy and challenging, spanning from the initial stage of laboratory bench research to clinical trials and, ultimately, the introduction of medications to the market (Figure 1). The identification of candidate medications is the hallmark of the two stages, and research and development are closely related. Benchwork enables us to identify the most promising compounds and subsequently enhance their performance [7]. The safety and efficacy of the tested pharmaceuticals can be determined through preclinical research and clinical trials. It is possible that a post-marketing surveillance trial or phase IV will be conducted to evaluate the safety of the drug after it has been approved for market use (Figure 1).

Research conducted in a laboratory

The primary stages of drug research are as follows: (i) target determination, (ii) model establishment, (iii) lead compound discovery, and (iv) lead compound optimization.

Establishment of desired outcome

This is the initial step in the new drug research and development process and the foundation for all operations that will be conducted to further select and determine the targets of human diseases. Upon the identification of drug targets, potential compounds or polypeptides are synthesized or modified, bioengineering products such as antibody/recombinant proteins are developed, and metadata analysis is employed to screen databases for novel druggable molecules [8,9]. Drug effects, chemical safety, and mechanism of action will be assessed in drug candidates.

The establishment of experimental models

Experimental models, including in vitro assays, in vivo assays, unique cell lines, binding affinity, kinetics, gene ablation, and transgenes, are required to screen and evaluate the biological and pharmacological activity of potential drug candidates after the target is selected [6,7,10]. In order to ascertain whether these drug candidates satisfy the action requirements and to guarantee the specificity of the research process, these experimental models are devised or adapted in accordance with the screening criteria and various tested compounds or other drug candidates [11].

The identification of lead compounds

The main compound is the one that is likely to be therapeutically druggable and possesses specific biological or pharmacological activity. Thousands of small molecule compounds are typically tested in laboratories with a variety of experimental methodologies and technologies to identify a lead compound that may target a unique gene, protein, or signaling pathway [7]. For example, the G Protein-Coupled Receptor (GPCR) family is of great importance in the field of drug
research and development. GPCRs are transmembrane receptors that interact with their ligands, which are generally considered to be potential medications. The ligand-receptor interactions and the associated models are essential for the discovery of the GPCR-targeting lead compounds. Extensive experimental screening and computational pre-screening, which are based on previously known structures and models, are the two primary methods for obtaining novel lead compounds [12].

**Lead compound optimization**

One of the most critical stages in drug research and development is the optimization of a lead compound. Optimization will be implemented to conduct additional assessments of drug potency, selectivity, toxicity, safety, molecule mechanism, and distribution after the identification of an initial lead compound [6]. The lead compound may possess certain defects or detrimental properties, including low action intensity or specificity, inappropriate pharmacokinetic properties, strong toxic side effects, or chemical or metabolic instability. The lead compound must be optimized, as it is incapable of being directly administered as a drug. For example, the compound’s chemical structure can be altered to decrease toxicity, increase potency, and enhance receptor specificity. The optimization process aims to create a series of compounds based on the principle of similarity, evaluate their exhaustive structure-activity relationship, and optimize their physical, chemical, and biochemical properties [6]. In summary, the objective is to achieve these objectives. Thereafter, the in vitro and in vivo activities are assessed.

**Clinical trials and preclinical investigations**

The preparation process, safety, dosage, acute and chronic toxicity, stability, formulation and components, pharmacokinetics, allergic reactions, efficacy, hemolytic and local irritation tests, mutagenicity, reproductive toxicity, carcinogenic toxicity, and other factors are assessed in preclinical studies following a series of in vitro and in vivo experiments to identify the most promising drug candidate and prior to drug clinical trials [1]. In order to evaluate the efficacy and safety of drug candidates on animals prior to clinical studies in humans, these evaluation experiments must be conducted by organizations or laboratories that are qualified with good laboratory practice (GLP) standards. These standards pertain to the management controls of non-clinical studies. Studies conducted in accordance with these GLP restrictions may be approved by the FDA for its new drug application.

**New prescription application under investigation**

The pharmaceutical company will be required to submit the appropriate investigational new drug application to the FDA for approval to commence human clinical trials upon the completion of the drug safety test [13]. The preliminary experimental results, methods, location, and the objects of further studies, the chemical structure of the compound, the mechanism of action in vivo, toxic side effects observed in animal studies, and the production process of the compounds should be included in the proposed new drug application. The new prescription
application must also undergo assessment and approval by the Institutional assessment Board. Afterward, the pharmaceutical company may commence human clinical trials with a phase I study. Annually, the FDA must receive at least one status report from the subsequent clinical investigations. Contract research organizations (CROs) are responsible for conducting human clinical trials, which typically encompass Phase I, II, and III [1]. In some cases, a post-marketing surveillance trial or phase IV trial may be extended to assess the drug’s safety and effects in the market.

**Clinical phase IV and new drug application**

The company will gather and evaluate all trial data during the third phase of the clinical trial before determining whether to submit a new drug application [14,15]. The FDA will cautiously assess all data from the phase III study and approve the company’s application if the company can demonstrate that their new drug is both safer and more effective than the comparable drug currently on the market. Physicians may prescribe the new medication upon its approval. The company is required to submit periodic reports to the FDA, which include all adverse reaction reports and certain quality control records. A phase IV study may be necessary to assess the drug’s long-term efficacy and adverse effects [16]. Phase IV clinical trials are less frequent than phases I, II, and III trials, despite the fact that they involve thousands of patients and last for years. The substance must be withdrawn from the market once severe adverse effects are confirmed [4]. The substance utilized in all clinical trials must be manufactured in accordance with Good Manufacturing Practice (GMP) standards to ensure its optimal quality. Consequently, it is crucial to implement effective business administration from the outset to the marketing phase.

Expected success possibilities, commercial attractiveness, market competitiveness, and identification of comparative advantages, as well as an assessment of success risk, litigation risk, cost risk, and other general considerations, are all necessary to determine whether or not to develop a drug. A significant portion of this is the responsibility of management and affiliated personnel, rather than the labor of R&D scientists.

**Pharmaceutical industry development trends and the current state of drug development**

The successful research and development of a novel substance can necessitate a significant amount of effort. In addition to the costly and time-consuming laboratory research, the three clinical trials (Phase I, II, III) typically require 15-18 years [17]. Consequently, drug research and development are significantly influenced by contemporary administration and management (Figure 2).

**Risk of drug research and development**

The research and development of new drugs is a project that must possess its own unique characteristics. As with any investment or research endeavor, there are inherent risks [1]. In the absence of complete assurance, it is imperative to allocate a substantial quantity of manpower and material resources to these
initiatives, thereby assuming substantial risks. Consequently, the project manager must exert considerable effort at the management level to mitigate the project’s hazards to the greatest extent feasible [18].

In 1997, the Asian financial crisis occurred, resulting in turbulence in the global financial industry. Risk prevention and management issues were increasingly examined in a variety of global sectors [19]. It is important for pharmaceutical companies and other operators to be aware that a single form of risk is frequently associated with others. Risk management is not limited to the management of a single risk within a single company, as it was in the past. It also encompasses the integrated management of all risks from the perspective of the entire system. The fundamental concept of comprehensive risk management is the implementation of all types of risk management by business entities at all levels of the organization. The high risk associated with drug research and development is unavoidable; however, the risks associated with these projects can be mitigated through the integrated implementation of mature management mechanisms in the pertinent disciplines [18,19].

Enhancing the oversight of drug safety

The entire society is deeply concerned about the safety of drugs and their potential adverse effects [4]. The use of antibiotics has been reported to lead to an increase in drug resistance. Consequently, the regulatory authorities overseeing drug safety have significantly enhanced their oversight. It is imperative that pharmaceutical enterprises enhance their internal management systems to prevent being overwhelmed by the evolution of the industry and to access additional resources and expand their capabilities. The revised draft of the “Standards for Quality Management of Drug Clinical Trials” that was implemented in China has been interpreted in a manner that plainly indicates that the mechanism of drug safety management has been further enhanced [20]. In addition to enhancing the supervision of clinical research on generic medications and electronic clinical trial data, the evaluation and supervision of third-party organizations have become more stringent. Simultaneously, there is an increased emphasis on conflict-of-interest management and information disclosure.

The operational mechanism in substance management has been enhanced and fortified by the appropriate regulatory bodies. This demonstrates that their clients, the regulated pharmaceutical enterprises, must enhance the innovation in pharmaceutical production and the gold content of its management, which has correlated with the increasing importance of the operation mechanism [20].

The significance of administration in preclinical and clinical trials

Laboratory management There are instances in which the laws that are in place during the drug development process are not adhered to, which poses a significant safety risk for the drug’s release. The development and research of a drug necessitates laboratory work, such as drug design, drug screening, and drug optimization. Laboratory management is indispensable in the process of drug development (Figure 2) [21]. In China, there are numerous categories of drug research and development institutions, including universities, research institutes,
and other drug research institutions. Among them, national research institutions and institutions of higher learning possess unmistakable advantages in terms of capital and policy, and their theoretical research and technical levels are among the highest in China. Nevertheless, the system and mechanism limitations have prevented the timely commercialization of excellent research accomplishments, and a significant portion of national capital input has been converted into academic papers rather than actual medicinal products [21].

The majority of pharmacological research institutions in China have not yet implemented an optimal quality management system. The research methods are not scientific, and the results are not true or reliable, as they lack effective and normative control of the research process and the supervision measures are imperfect. At present, international laboratories depend on a laboratory accreditation procedure as an impartial assessment of their capabilities. The professional and technical assessor evaluates all the factors that effect the data in an organization on the basis of the international standard ISO/IEC17025, and the evaluation criteria are consistent with this standard. However, only a handful of laboratories in the field of drug research in China have been accredited to date, and the primary laboratory is a pharmacological research laboratory [21].

Consequently, it is recommended that the international standard ISO/IEC17025 and the IS 9000 series quality management system be consulted in order to establish the criteria for evaluating the capabilities of pre-clinical research laboratories in our country and to assess the capabilities of the laboratories by third-party organizations. In order to encourage the active management of pre-clinical research laboratories (Figure 2) and fully realize their primary responsibility, we should implement certain preferential policies in the pertinent administrative examination and approval processes [4,21]. For example, we should expedite the evaluation process.

**Management of drug testing**

Substance testing is the process of utilizing a substance or a placebo as a control or trial in a clinical trial. In order to safeguard the rights and interests of the subjects, it is crucial to enhance the management of the test medications due to the degree of uncertainty regarding their safety and efficacy [4]. The foundation for guaranteeing the accuracy and dependability of clinical trial data is the establishment of a comprehensive drug management system and the enhancement of the entire drug research process management (Figure 2) [22]. At present, the drug management patterns of clinical research are primarily categorized into three groups: the management model of the professional group (which has been rarely employed), the joint management model of the organization and the professional group, and the management mode of the pharmacy of the clinical research center. The conventional approach to substance management involves institutional supervision and professional possession. The professional group's drug administrators are accountable for the receipt, custody, distribution, and recovery of drugs. The management mode is plagued by numerous issues, including the absence of specialized securing containers for the maintenance and preservation of management records and documents, as well as the absence of punctual temperature and humidity records in the professional
group. The safety of the subjects cannot be completely guaranteed, and it is easier to regulate the temperature and humidity of drug storage or to prevent non-test subjects from obtaining the research drugs. Consequently, the future will see the emergence of a centralized management system for experimental medicines [22,23].

The primary components of drug use management are the receipt of confirmation, registration, storage and protection, use, recovery, and disposal of drugs and records. The quality of the test medications and the efficient use of the drug in clinical trials can only be guaranteed by adhering to these steps and exercising rigorous management in accordance with relevant professional regulations. The office of clinical trials of drugs, as a quality management department of clinical trials, is responsible for the establishment of a management system that is in accordance with the agency’s current circumstances. This system is designed to guarantee the scientific, reliability, and authenticity of the test results, thereby enhancing the overall quality of clinical trials in our country [4,22].

The management of experimental drugs is a meticulous and laborious process. GCP, pertinent systems, and test plans must be adhered to by each link. In the context of drug clinical trials, any unstandardized link in drug management can result in dubious results for the trials and even jeopardize the safety of the subjects and patients after the drug is launched (Figure 2). The management of experimental drugs should be of paramount importance to all parties involved in clinical trials, including the applicant, the researcher, and the contract research organization (CRO), in order to ensure that the management of each link is standardized, thereby obtaining scientific and reliable experimental data and safeguarding the safety of the subjects [24].

Project administration for clinical trials

Experts, patients, businessmen, administrators, coordinators, and other participants from various disciplines are all involved in drug R&D administration. Project management is applicable to one-time duties that require significant investment, complex relationships, and limited time and resources. Project management is also necessary for the research and development of new drugs. The research and development of novel medicines is a rigorous and intricate process. A sequence of procedures, including synthetic extraction, biological screening, pharmacology, toxicology, and other preclinical studies, formulation and stability experiments, bioavailability tests, amplification experiments, and the necessity of human clinical trials, is required to progress from laboratory research to the launch of a new drug. Registration, launching, and after-sales supervision are among the numerous intricate connections. Effective project management is a critical factor in the success of a project, particularly in the context of complex and extensive system engineering. Nevertheless, the research and development of new pharmaceuticals in China have not been the subject of systematic and mature project management, particularly in the context of clinical trials that involve the safety of human medications. The researchers’ cognizance and concern regarding project administration are inadequate. Consequently, it is of the utmost importance to enhance the implementation of project management in the clinical trials of new drugs [4,25].
In recent years, project risk management has garnered increasing attention from pertinent personnel, particularly due to the product particularity of novel drug clinical trial projects, which renders the project's risk factors complex and subject to change. Consequently, it is imperative to prioritize risk management awareness, establish risk assessment and decision-making processes, and mitigate or lessen the impact of risk during the project management process. Furthermore, the success of project management is ensured by the establishment of an effective performance evaluation system and the strengthening of the human resource management of the project stakeholders, as the new drug clinical trials involve a significant number of stakeholders [25].

The value of project management is widely acknowledged by technicians and managers, who employ it to ensure that a project is executed to the highest standard. The practice has demonstrated that the application of project management in the process of new drug clinical trials is of great significance for enhancing the efficacy of R&D and the capacity of enterprises to conduct new drug research and development [26]. The formulation of plans, the determination of "milestone events," the control of the process, the termination of the project, and the management of the project team are of great guiding significance to novel drug developers in the project management system. In addition, numerous project process control chart tools in project management knowledge systems are of greater practical and direct importance for the research and development of new drugs [25,26].

**Data administration**

One of the most critical components of safeguarding the rights and safety of participants in clinical trials is the safety monitoring of experimental data. The fundamental responsibility of GCP institutions is to guarantee the accuracy, completeness, and traceability of test data in order to adhere to CFDA policies and regulations. GCP institution administrators, researchers, applicants, quality monitors, auditors, and others are among those accountable for monitoring (Figure 2). In the process of drug development, the quality of the process can be enhanced by enhancing data management. This can also facilitate the rapid integration of data, the identification of issues, and the enhancement of the development data of more scientific systems during the drug certification phase. Consequently, it is imperative to implement effective data management [12,26]. The implementation of electronic data management systems has become the popular trend in recent years. Electronic data capture (EDC) is a critical measure for guaranteeing the quality of clinical trials for novel drugs. It has the potential to enhance the applicant's monitoring of the research, reduce the time to data acquisition and administration, increase the accuracy of data collection, and enhance the overall efficiency of R&D [12,25,27]. In order to generate more substantial economic advantages, drug research and development programs frequently allocate funds to two or three electronic data management systems.

**Drug production management is mandated by the FDA.**

An FDA official conducts an onsite GMP conformity inspection of the manufacturer and the entire drug production chain to guarantee the quality of
the produced drugs after the registration of the new drug's DMF document is finalized with the application of the drug in the United States [26]. The FDA's decision to approve raw materials for the US market is based on an on-site inspection. In the United States, GMP is distinguished by its timeliness and dynamic nature. The emphasis is on the current GMP, and the entire production, quality control, logistics, and facilities and equipment process must be verified [26,28]. The GMP procedure is also traceable and elucidating, and its regulations in the United States are generally regarded as the most stringent in the world. In contrast, FDA officials are extremely serious about on-site inspections, and the agency's requirements for Chinese API manufacturers are exceedingly stringent. There are numerous domestic manufacturers that have obtained FDA approval.

The FDA conducts a thorough and significant inspection of the production process, from the unprocessed material to the finished products. The results of the operation conditions, methodologies, and equipment of certain critical stages in the process are typically closely monitored. The FDA believes that the prerequisite for guaranteeing the quality of the products is the validation of the production process. From the pilot stage to the full industrial scale, a comprehensive verification system must be implemented for a new product. The production process that has been implemented for an extended period of time necessitates retrospective verification. In general, the substantiation of the production process is not permanent, and any modification should be acknowledged. Furthermore, each process and operation of the production are governed by standard operating procedures (SOPs), which encompass the warehousing, inspection, and distribution of basic materials, as well as the quality control and operation management [26,29].

**Pharmaceutical companies' cooperative management mechanisms**

Foreign pharmaceutical companies are involved in the drug discovery and development process in the areas of metabolism, cancer, and immunology in various disease areas, as well as small molecular medicines, by utilizing computational chemistry technology [30-33]. In the realm of computer-assisted drug development, the Nimbus Therapeutics Company has established a close partnership with the Schrödinger Company to create customized procedures [34]. In order to establish a profound integration between drug discovery and computer technology, the joint teams of the two companies design, iterate, optimize, and support the rapid iteration and refinement of novel methods [11]. The most recent developments in human genetics and biology are closely associated with the selection of drug targets that address unmet clinical requirements, when combined with computational chemistry. Simultaneously, the organization has established an effective management system and collaborated with academia and industry to advance the development of new drugs [35,36]. The company concentrates on three physiological mechanisms that intersect in the field of drug development: metabolic disorders, malignancies, and immune disorders. The connections between these three diseases are currently being elucidated [37,39]. A variety of metabolic system diseases, including nonalcoholic steatohepatitis and type I diabetes, can be caused by an overactive immune system. In recent years, it has emerged as a significant medical advancement in the field of tumor immunotherapy, which involves the use of the immune system to combat and
eliminate tumor cells. Targeted tumor cell drug molecules can also be identified by identifying physiological metabolic pathway differences between tumor cells and normal cells.

**Data management system**

Technology (algorithms) and data are the two components of AI. Currently, the most significant obstacle encountered by the medical industry AI is the scarcity of data. The majority of international artificial intelligence algorithms are open source software; a new algorithm will soon be converted into a convenient module, ensuring that the data is not a bottleneck, but the AI technology is [11]. The primary challenge in the field of AI research in medicine is the absence of high-quality and clear clinical labeling of critical data. In order to address this issue, government agencies, including the Food and Drug Administration (FDA), the Institute of Health, large hospitals, and medical technology companies, can collect a substantial quantity of high-quality data. This will significantly advance the field of AI in medical applications [34,36,37]. For instance, lumina, a major manufacturer of sequencing instruments and a gene screening testing company, collects the genetic and clinical characterization data of 20,000 tumors. This data is of significant assistance in the implementation of artificial intelligence in precision tumor treatment [39].

**Summary**

Drugs become increasingly effective and diverse as drug research and development progresses and the development mechanism becomes more innovative. At the same time, the supervision and administration of drug research and development are becoming increasingly difficult. Consequently, in order to foster the advancement of the pharmaceutical industry and mitigate the risk of enterprise development, it is imperative to integrate the research and development of new drugs with an innovative management system, optimized management structure, and integrated innovation of management modes into scientific research. The economic value of drug research and development and the benefits to human health will be improved as a result of these measurements.

**References**


Figure 1. The process of drug research and development
Figure 2. Management is engaged in a variety of drug research and development fields.