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A Review on Artificial Intelligence in Pharmaceutical Science

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Abstract: ***In recent years, the use of artificial intelligence (AI) in health care has risen steadily, including a wide range of applications in the field of pharmacology. AI is now used throughout the entire continuum of pharmacology research and clinical practice and from early drug discovery to real-world data mining. The types of AI models used range from unsupervised clustering of drugs or patients aimed at identifying potential drug compounds or suitable patient populations, to supervised machine learning approaches to improve therapeutic drug monitoring. Additionally, natural language processing is increasingly used to mine electronic health records to obtain real-world data. In this mini-review, we discuss the basics of AI followed by an outline of its application in pharmacology research and clinical practice. Artificial intelligence is the upcoming technology in advance health care system. Current digitalization of medicine and availability of electronic health records (EHRs) has inspired clinical researchers and healthcare personnel to acquire artificial intelligence (AI) methodologies for big data analytics and for very large scale medical databases. The major advantage of AI is that it reduces the time that is needed for drug development and, in turn, it reduces the costs that are associated with drug development, enhances the returns on investment and may even cause a decrease in cost for the end user. A large number of researches are being carried out to improve the current available AI technology to make the pharmacy profession more efficient. The present article briefly describes the importance of AI in the process of drug development and then looks at the various AI tools that are available at the disposal of a modern-day pharmacist to aid in a more efficient functioning.***

Keywords: Artificial Intelligence, Drug discovery, Robotic Pharmacy, Technology and Tools, Machine learning, Deep learning.

I. INTRODUCTION

The Artificial Intelligence (AI) deals with interpreting information and analyzing the application of algorithms. Advanced computer algorithms are used in AI to perform tasks like humans such as making decisions and data interpretations. AI provides different options to identify various problems and to solve the Like human beings, machines of AI, have critical thinking capacities. AI functions through a number of routes, permitting systems to detect new patterns and different formulations are derived with given data It is an important part of artificial intelligence and is frequently used in medicine. From a very complex sets of analytical data ANN can recognize various patterns, thus it becomes very convenient in data analysis of pharmacological research for their capacity to identify non-linear relationships from random data. [1] AI in healthcare has evolved dramatically over the last five decades, leading to significant advancements in a variety of medical fields. The introduction of ML and deep learning (DL) has expanded AI applications, enabling personalized medicine rather than relying solely on algorithms. AI has significantly impacted clinical decision-making, disease diagnosis, as well as clinical, diagnostic, rehabilitative, surgical, and predictive practices. This advancement in AI technology has paved the way for improved diagnostic accuracy, streamlined provider workflow, improved clinical operation efficiency, disease, and therapeutic monitoring, precise procedures, and, ultimately, better patient outcomes.[2] Structure activity relationship (SAR) of natural atoms was studied by Klopman. The program implied for structure assessment is PC mechanized, and it perceives structures of atoms from the KLN code, which is a straight coding daily practice of the atom, consequently and at that point further recognizes, arranges, and breaks down biospheres, which are substructures that are really answerable for the natural action of the particles, measurably. Inside the computerized arrangement of the drug store, the PCs first get drug arranges electronically from the doctors and drug specialists of UCSF. After this, person dosages of pills are picked, bundled, and administered by the mechanical technology. [3]

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AI is a stream of science related to intelligent machine learning, mainly intelligent computer programs, which provides results in a similar way to the human attention process. This process generally comprises obtaining data, developing efficient systems for the uses of obtained data, illustrating definite or approximate conclusions, self-corrections, and adjustments. In general, AI is used for analyzing machine learning to imitate the cognitive tasks of individuals. AI technology is exercised to perform more accurate analyses as well as to attain useful interpretation. In this perspective, various useful statistical models, as well as computational intelligence, are combined in AI technology.[4] Artificial Intelligence (AI) is the branch of engineering science which deals with making of intelligent machines, especially intelligent computer programs. It is the ability of a computer or a robotic computer enabled system to process the given information and produce outcomes in a manner similar to the attention process of humans in learning, decision making and solving problems. AI is a branch of computer science that aims to create intelligent machines, which becomes an essential part of the technology industry. Research associated with AI is highly technical and specialized. [5] In healthcare the most common place where machine learning is used is precision medicine. Precision medicine is predicting what treatment protocols will success on a given patient, and this is determined based on past data of patients. [6]

II. APPLICATIONS OF AI IN PHARMACOLOGY

In the application of machine learning, deep learning methods (e.g., convolutional neural network), and natural language processing AI has brought about a ground breaking transformation in various stages of drug discovery, development (including the discovery phase, clinical trial phase, and post-marketing surveillance) and precision medicine.

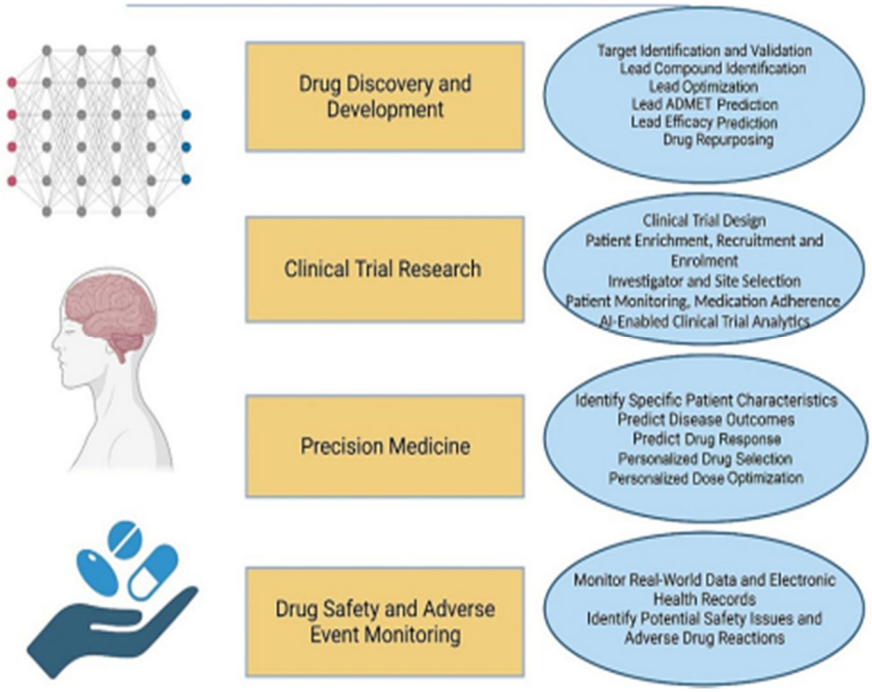


Fig. 1: Application of artificial intelligence in pharmacological research and precision medicine.

Utilizing machine learning, deep learning (CNN) techniques, and natural language processing AI has revolutionized drug discovery and development (discovery phase, clinical trial phase, and post-marketing surveillance) and precision medicine. [7]

III. TOOLS OF AI

A. Robot Pharmacy

The objective of improving the safety of patients, UCSF Medical Center uses robotic technology for the preparation and tracking of medications. According to them, the technology has prepared 3,50,000 medication doses without any error. The robot has proved to be far better humans both in size as well as its ability to deliver accurate medications. The abilities of the robotic technology include preparations of oral as well as injectables medicines which include chemotherapy drugs that are toxic. This has given freedom to the pharmacists and nurses of UCSF so that they can utilize their expertise by focusing on direct patient care and working with the physicians.

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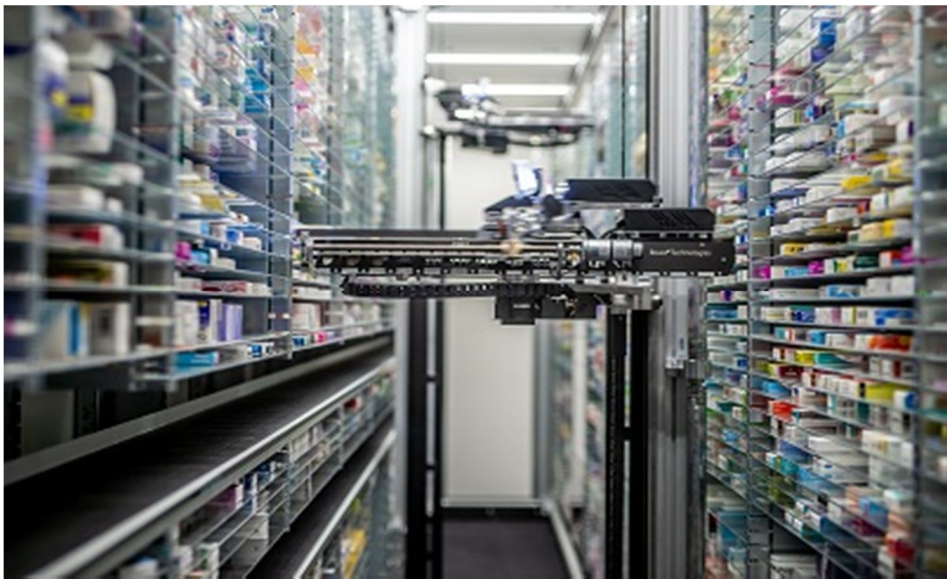


Fig. 2: Robotic Pharmacy. [8]

In AI, machines imitate critical thinking capabilities with other human personalities. As of now, most of the applications of AI are primitive as they are designed to do limited tasks and to a limited extent. AI works through multiple paths, allowing systems to discover new patterns and derive their own rules when given with data and new experience. Some of the critical applications of AI in pharma are designing treatment plans, checking the accuracy of medicine and in drug creation. Major pharma companies are adopting AI software or partnering with AI-based start ups to accelerate drug discovery. With AI, customization of dosages can be achieved based on individual patient characteristics. AI is also increasingly being used to detect drug effectiveness and to understand adverse drug events. It may also help accelerate drug approval processes by the regulatory authorities. [10]

B. MEDi Robot

MEDi is a short form for Medicine and Engineering Designing Intelligence. The pain management robot was developed as part of a project led by Tanya Beran, professor of Community Health Sciences at the University of Calgary in Alberta. She got the idea after working in hospitals where children scream during medical procedures. The robot first builds a rapport with the children and then tells them what to expect during a medical procedure. During the medical procedure, it guides them on what should be done, how to breathe during the procedure, and how to cope. Although the robot cannot think, plan, or reason, it can be programmed such that it shows to have AI.



Fig. 3: MEDi Robot

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MEDi, manufactured by Aldebaran Robotics, having inbuilt facial recognition technology, can speak 20 different languages and is highly adaptable to different situations. The retail price of the robot is $9000; however, the cost rises to $15000–$30000 when the applications needed for the robot to help in medical procedures are installed. The robot was initially developed for pain management, but with time its use has expanded to comfort between procedures, physical rehabilitation, and fundraising. The robot first builds a rapport with children scream during medical procedure. During the medical procedure, it guides them on what should be done, how to breathe during the procedure, and how to cope. Although the robot cannot think, plan, or reason, it can be programmed such that it shows to have AI. [8, 12]

C. ERICA Robot

Erica is a new robot created by Hiroshi Ishiguro, a professor at Osaka University in Japan. It was developed in collaboration with the Japan Science and Technology Agency, Kyoto University and the International Advanced Telecommunications Research Institute (ATR). He speaks Japanese and has a mixture of European and Asian facial features. Like any normal person, he loves animated movies, wants to travel to South Asia, and wants to spend his life with someone he can talk to. The robot cannot walk on its own; but has developed the ability to understand and answer questions using human facial expressions, a robot nose, eyes, etc. has created. The Erica robot pharmacy developed by a company called Erica Technologies is an advanced robotic system designed to automate various tasks within a pharmacy setting. This technology aims to streamline prescription dispensing, inventory management, and customer service in pharmacies.



Fig. 4: ERICA Robot [13]

IV. CHALLENGES THAT PHARMA COMPANY'S FACE WHILE TRYING TO ADOPT AI

1) The unfamiliarity of the technology – for many pharma companies, AI still seems like a "black box" owing to its newness and esoteric nature.

2) Lack of proper IT infrastructure that's because most IT applications and infrastructure currently in use weren't developed or designed with artificial intelligence in mind. Even worse, pharma firms have to spend lots of money to upgrade their IT system.

3) Much of the data is in a free text format – that means pharma companies have to go above and beyond to collate and put this data into a form that's able to be analyzed. Despite all these limitations, one thing is for certain: AI is already redefining biotech and pharma. And ten years from now, Pharma will simply look at artificial intelligence as a basic, everyday, technology.



Fig. 5: Challenges to adoption of AI in pharma. [14]

The implications of AI in pharmacy apps for people at homes are immense, providing several advantages to users. With AI integrated into pharmacy apps, users can access medical advice, medication information, and guidance on dosage and usage from the comfort of their homes. This can be especially beneficial for people with mobility issues or those living in remote areas. AI can also analyze a user's medical history and help develop personalized medication regimens, including dosage, frequency, and timing, ensuring that users are taking their medications correctly and effectively. With AI integrated into pharmacy apps, users can receive 24/7 support for any medication-related queries or concerns, eliminating the need to wait for a pharmacist's office.[15] He dawn of the 21st century, however, introduced a paradigm shift in this quest. As we tread deeper into the age of information, two formidable entities have emerged at the forefront of numerous industries, including health care and pharmaceuticals: artificial intelligence (AI) and big data. While these terms have permeated virtually every domain, their implications in drug discovery are profound, promising a revolution in the ways drugs are researched, developed, and brought to market. [16]

V. ROLE OF AI I PHARMACEUTICAL INDUSTRY:

Artificial intelligence (AI) has a significant role to play in the pharmaceutical industry when it comes to addressing various challenges. Using AI algorithms, extensive biological data can be analysed in order to identify targets that are associated with diseases, as well as predict how these targets interact with potential drug candidates .This allows for a more efficient and targeted approach to the process of drug discovery. Machine learning algorithms also contribute by assisting in the design of experiments, predicting pharmacokinetics and toxicity, and optimizing lead compounds. As a result, the need for extensive animal testing is reduced. Moreover, AI algorithms can analyse real- world patient data, which in turn facilitates personalized medicine approaches. [17] This review provides an overview of the current developments and AI technologies used in drug discovery and design, clinical trials, precision medicine and pharma-covigilance. It is crucial for the researchers from various fields that collaborate with pharmaceutical specialist's to have the knowledge on the current AI tools used in pharmaceutical medicine. [18] Artificial intelligence has attracted many users over the past, it supports medical sciences, businesses, scientific researches etc. These systems when implemented with great cautions, gave surprisingly accurate results and avoided errors likely happened by humans. These systems never falter because they follow a specific track to achieve a goal by using the information provided. In case if we don't have enough knowledge for designing some system, system is provided with past knowledge base to develop itself and make decisions on that knowledge base. [19] Healthcare has lately relied on AI. AI has improved healthcare. "Will AI replace Doctors inthe future?" is also debated. It's unlikely soon. It aids regional clinical decision-making. The expanding availability of medical care information and the quick development of massive data investigation tools have helped appropriate AI applications in medical services. When driven by appropriate clinical queries, practical AI algorithms may locate clinically usable information in enormous volumes of data, aiding clinical decision-making Doctors and health administrations under tremendous strain due to changing demographics, logistical demands, faculty shortages, rising morbidity, and data innovation interest and standards. [20]

A. Artificial Intelligence in Research and Development

Pharma companies all over the world are streamlining the drug development process with cutting-edge machine learning algorithms and AI-powered platforms. As a result of their ability to recognise complex patterns in vast datasets, these intelligent technologies can be utilised to address problems relating to sophisticated biological networks. This ability is great for analysing the patterns of different diseases and figuring out which drug formulations would be most effective for treating particular characteristics of a given condition. The development of medications with the best odds of curing an illness or other medical condition can thus be funded by pharmaceutical corporations. [21]

B. Robot Assisted Surgery

Robotic surgery, computer-assisted surgery, and also robotically-assisted surgery are terms for technological improvements that utilize the robotic systems to assistance in surgical procedures. The most familiar surgical robot is the da Vinci Surgical System. Recently, Google has reported that it commenced working with the pharmaceutical giant Johnson& Johnson in designing a new surgical robot system. Robotically-assisted surgery was created to beat the limitations of advance minimally-invasive surgical procedures and to improve the capacity of surgeons performing open surgery. In the case of robotically assisted minimally-invasive surgery, instead of straightly moving the instruments, the surgeon uses one of two methods to control the instruments; either a direct telemanipulator or through computer control. . One beneficial use of the the computerized technique is that the surgeon does not need to be available during the surgery, but rather can be anywhere in the world, top to the likelihood for remote surgery. They are not the only revivals, though. With their AXSIS robot, Cambridge advisers aspire to conquer the limitations of the da Vinci, such as

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its big size and inability to work with extremely detailed and delicate tissues. Their robot somewhat relies on flexible components and small, worm-like arms. The programmer consider it can be applied later in ophthalmology, e.g. in cataract surgery A telemanipulator is a remote controller that allows the surgeon to execute the ordinary activities related with the surgery in the meantime the robotic arms complete those movements using end-effectors and manipulators to do the real surgery on the patient. In computer-controlled systems the surgeon utilizes a computer to deal with the robotic arms and its end effectors, however these systems still utilize telemanipulators for their information.



Fig. 6: *AI-assisted Robotic Surgery. [22]*

C. AI Support Antibiotic Study

Antibiotic discovery has become more complicated in recent years with the rise of antibiotic resistance. Earlier, antibiotics were discovered by screening soilswelling microbes for secondary compounds prohibited bacterial growth. However, antibiotic development is currently hampered by the discovery of the same molecules repeatedly. Recently, a study showcasing machine learning to find new antibiotics was released, where researchers employ machine learning to anticipate antibacterial chemicals in silico from a database of over 107 million molecules. This antibiotic, known as "Halicin," is effective against various bacteria, including tuberculosis and difficultto-treat types. Other medications could benefit from this strategy, such as those used to treat cancer or neurological illnesses. [23]

This intelligency of machine has made life smoother and more comfortable than ever expected. One cannot restrict this programmed machine or software to mentioned areas. It has stretched its legs towards health system, particularly, pharmaceutical sciences. Followings are the areas of pharmaceutical science where AI can be employed.

1) Pharmaceutics which mainly deals with formulations and development of drugs, manufacturing of dosage forms.
2) Pharmaceutical chemistry, a branch deal with structure, chemistry, analysis of medicines.
3) Pharmacology discipline involve with animal study, toxicity study and clinical study.
4) Pharmacognosy is a science comprise of study of natural products chemistry and its applicability to cure disease. [24]

VI. AI FOR PHARMACOKINETICS AND PHARMACODYNAMICS:

Drug development is a complex process that involves several stages, including drug discovery, preclinical studies, clinical trials, and regulatory approval. Pharmacokinetics and pharmacodynamics are crucial aspects of drug development, as they determine the optimal dosage, administration route, and safety of a drug in the body. Traditional experimental methods for pharmacokinetics and pharmacodynamics studies can be timeconsuming and expensive and may not always provide accurate predictions of drug efficacy and safety. Traditionally, pharmacokinetics and pharmacodynamics studies have been conducted using experimental methods such as animal studies and human clinical trials. These methods have critical challenges, such as ethical concerns, sample size, and inter individual variability.

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Furthermore, these studies may not always provide accurate predictions of drug pharmacokinetics and pharmacodynamics in humans. [25] Doctors don't have to learn by heart almost as much more data as they did 50 years before. Digital technology has liberated medical doctors, nurses and researchers to focus further mental energy on higher-level cognitive tasks and patient concern. AI is ready to obtain this to the next stage. „Thinking" time was spent getting into a position to think, to build a decision, to study something. Much more time went into discovering or acquiring information than into digesting it. More than a few hours of calculating were required to obtain the data into comparable form. When they were in comparable form, it took only a only some seconds to decide. [26] Metabolism and excretion are two important processes in pharmacokinetics overview of drug metabolism and excretion. Metabolism is the biological transformation by which most drugs undergo a change in their chemical structure in the body to produce the expected therapeutic effects of a certain drug and be more easily eliminated from the body. Drug excretion refers to the elimination of drugs or their metabolites from the body Drug metabolism can yield metabolites that differ greatly from the original drug's physical and pharmacological characteristics. The rate of metabolism dictates the length and strength of a drug's pharmacologic effect. Drug metabolism also plays a role in multidrug resistance in infectious illnesses and cancer chemotherapy, and the effects of certain medications as inhibitors or substrates of enzymes involved in xenobiotic metabolism are frequent causes of adverse drug interactions. Drug metabolism affects drug efficacy and toxicity in humans and laboratory animals. Metabolism is also responsible for the clearance of more than 70% of clinical medicines so it has been extensively researched as part of drug research and development (R&D) efforts. Both metabolism and excretion are tightly regulated by the body to maintain homeostasis and ensure that harmful substances are eliminated from the body. [27]

VII. LIMITATIONS AND FUTURE PERSPECTIVES

Despite the enormous advancement of AI in the advancement of drug discovery and innovation, the lack of accountability might hinder this technology as it is claimed to produce false information and safety concerns by generating threatening content. In addition, the automation of special tasks can lead to job displacement; however, augmented capabilities of humans pave the way for new job opportunities and productivity enhancement. Implication of AI may also encounter ethical issues regarding bias and data privacy. Hence, considerable care should be taken for the data used to train the model; nevertheless, AI/ML has no ethical concern for drug development. [28]

VIII. ADVANTAGES OF AI TECHNOLOGY:

1) *Error Reduction:* AI, or Artificial Intelligence, plays a vital role in improving the efficiency of various processes by minimizing errors and increasing accuracy. Intelligent robots are designed with strong metal bodies, making them capable of enduring harsh conditions in space. As a result, they are chosen for space exploration missions
2) *Medical Application:* Physicians are now using artificial intelligence to screen patients and analyze health concerns. The AI program educates physicians on numerous medications and their side effects
3) *Difficult Exploration:* AI demonstrates its valuable applications in the mining industry and proves equally beneficial in fuel exploration. Additionally, AI systems play a crucial role in oceanic exploration by effectively mitigating errors caused by human intervention
4) *Daily Application:* AI is quite useful in our daily actions and activities. GPS, for example, is widely utilized in long-distance driving. AI installation on Androids aids in predicting what a person would type. It also aids in the repair of spelling errors. For Ex- Lady SIRI
5) *Digital Assistant:* Modern organizations employ AI systems, like digital assistant 'avatars,' to minimize human dependency. These avatars make logical decisions without being influenced by emotions. Unlike humans, emotions don't impact their judgment, resulting in more efficient decisionmaking and problem-solving. Machine intelligence helps overcome the limitations of human emotions and enhances overall effectiveness.[11]

IX. DISADVANTAGES OF AI TECHNOLOGY:

The important disadvantages of AI technology are as follows

1) *Expensive:* The launch of AI causes huge money consumption. Complex designing of machine, maintenance and repairing are highly cost effective. For the designing of one AI machine, a long period of time is required by the R&D division. AI machine needs updating the software programmes, regularly. The reinstallations as well as recovery of the machine consume longer time and huge money.

2) *No Replicating Humans:* Robots with the AI technology are associated with the power of thinking like human and being emotionless as these add some advantages to perform the given task more accurately without any judgement. If unfamiliar problems arise, robots cannot take the decision and provide false report.
3) *No Improvement with Experience:* Human resource can be improved with experiences. In contrast, machines with AI technology cannot be enhanced with experience. They are unable to identify which individual is hard working and which one is nonworking.
4) *No original creativity Machines with AI Technology:* have neither sensitivity nor the emotional intelligence. Humans have the ability to hear, see, feel and think. They can use their creativity as well as thoughts. These features are not achievable by the uses of machines.
5) *Unemployment:* The widespread uses of AI technology in all the sectors may cause large scale unemployment. As because of the undesirable unemployment, human workers may lose their working habits and creativity. [9]

X. CONCLUSION

The use of artificial intelligence (AI) in healthcare, particularly in the field of pharmacology, has seen significant growth in recent years. AI is now integrated across various stages of pharmacology research and clinical practice, from drug discovery to real-world data mining. Its applications range from unsupervised clustering to supervised machine learning, enhancing therapeutic drug monitoring and precision medicine. AI tools like machine learning, deep learning, and natural language processing have revolutionized drug development, clinical decision-making, disease diagnosis, and patient outcomes. The adoption of AI in pharmacy settings, such as robot pharmacies and pain management robots like MEDi, showcases the potential for improved patient care and medication management. Despite challenges like unfamiliarity with the technology and data formatting issues, AI is reshaping the pharmaceutical industry by streamlining drug development processes and enhancing pharmacokinetics and pharmacodynamics studies. Overall, AI in healthcare, especially in pharmacology, holds immense promise for advancing medical research, improving patient care, and optimizing drug development processes.

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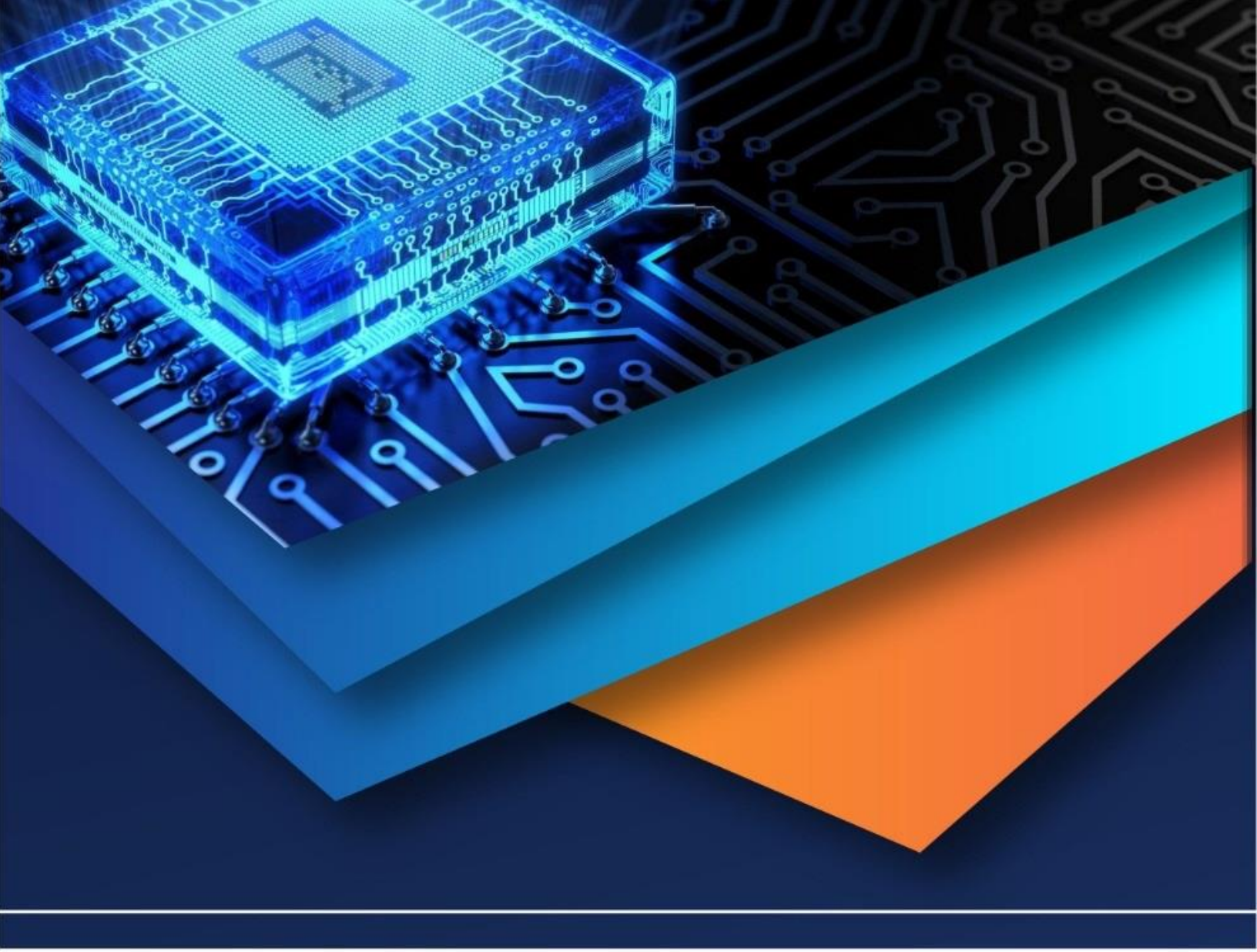
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