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AI in Drug Development: Applications and Challenges

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Abstract: ***The drug discovery process is a long and complicated one, involving multiple steps and issues, starting from target identification and ending with clinical development. The amount of chemical, biological, and clinical data produced by modern pharmaceutical companies is tremendous, and there is a continuous need to develop new approaches that could allow for efficient data mining and identification of relevant information. In this regard, artificial intelligence (AI), and specifically machine learning (ML) and deep learning (DL) seem to be an attractive choice for researchers for tackling the challenging task of data analysis.***
In silico artificial intelligence has been applied at all stages of the drug discovery and development pipeline, ranging from molecular target identification, virtual screening, molecular docking, quantitative structure-activity relationship, ADMET prediction, de novo design, ligand and lead optimisation, computer-assisted synthesis design, drug repurposing, and clinical trials.
These approaches can facilitate the exploration of large data sets and the prioritisation of compounds for experimental assessment, thereby reducing the time and cost associated with traditional drug discovery. and expensive traditional drug discovery.
However, despite the reported benefits and opportunities, there are still some limitations associated with AI-driven drug discovery, including dependence on large data sets with diverse characteristics, insufficient data for model training, data bias, overfitting, lack of interpretability, absence of independent evaluation, and regulatory issues.
Therefore, it is essential to view AI technologies as an instrumental but supplementary part of decision-making in pharmaceutical research and development rather than a fully independent alternative to traditional hit- and lead-discovery strategies The manuscript is a Review article that focuses on the main areas of application of artificial intelligence for drug discovery and development, including benefits, drawbacks, ethical issues, and opportunities.
Keywords: Artificial intelligence; Machine learning; Deep learning; Drug discovery; Virtual screening; Molecular docking; QSAR; ADMET; De novo drug design; drug repurposing, novel drug discovery.

I. INTRODUCTION

Drug discovery conventionally comprises a series of experimental and *in silico* processes for detecting molecules exhibiting desired or improved therapeutic activity, selectivity profile, pharmacokinetics and safety. The drug discovery process typically involves target identification, hit discovery, lead optimisation, preclinical and clinical development, each of which is associated with significant scientific and financial investment and entails a considerable level of uncertainty. [1,2,3]

Pharmaceutical research and development have seen data explosion and exponential growth of chemical, genomic, proteomic, electronic health records, and other databanks due to an unprecedented amount and diversity of information needed in modern drug discovery for significantly different types and complexity of databases currently being used in the field, necessitating standardized methods of accessing information from these resources. The use of artificial intelligence and machine learning seems promising in the task of interacting with databases of this kind and obtaining valuable data through their analysis or patterns that may not be apparent at first glance. [4,5,6]

Indeed, computational approaches have been used in pharmaceutical R&D for decades and contributed to quantitative structure-activity relationship (QSAR) analysis, chemogenomic, molecular docking, and predictive toxicology, among other applications. The convergence of increased computational power, availability of diverse data sets, and advanced machine learning algorithms have created an unprecedented opportunity to propel and advance drug discovery and development. [7,8,9]

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Recent studies have demonstrated the ability of artificial intelligence to support applications across different stages of the drug discovery process, from target identification to drug design and development. [2,4,7] Moreover, the emergence of deep learning and generative models has enabled the in-silico prediction of key molecular properties and the design of novel drug molecules with desirable characteristics. [7,9,10]

The present review seeks to discuss the role of artificial intelligence in drug discovery and development to emphasize the challenges and opportunities that need to be considered for the effective implementation of this innovative technology in pharmaceutical R&D.

II. ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY

Artificial intelligence is usually defined as a branch of computer science devoted to the development of algorithms that excel at performing tasks requiring human intelligence such as learning, reasoning, perception, decision making and so on. In drug discovery, AI is applied to analyse chemical or biological information and predict properties or interactions that are of interest for pharmaceutical purposes. [2,4,7]

Machine learning is the mainstay of most AI applications where algorithms are trained to extract information from a previously acquired data set in order to build predictive models. For drug discovery, applications include predicting chemical properties, screening libraries of compounds, analysing biological information as well as designing drug molecules. There are several variations of this approach that are used depending on the type of problem addressed. These include supervised learning, where positive and negative examples are used to train the algorithm, unsupervised learning which uses unlabelled data and reinforcement learning where an agent learns to make decisions based on rewards and punishments. [8,9,11]

Deep learning is a family of multilayer neural-network methods that can learn hierarchical representations directly from data that enables the computer to learn hierarchies of information directly from the data. It has found several applications in drug discovery including deep learning methods for molecular property prediction, virtual screening, de novo molecular design and other applications. [7-9,12]

However, success with AI applications in drug discovery requires more than just using better algorithms. Some of the other factors that contribute to model performance include the quality of the input data, representation of the information, choice of features and proper evaluation. [5,6,13]

III. NEED FOR AI IN DRUG DISCOVERY

A. Large and Complex Datasets

Due to the variety of sources of data about chemical libraries, biological tests, genomics, proteomics, and clinical trials, contemporary pharmaceutical research produces an expanding amount of information. The combination of these datasets allows studying the properties of drug targets and candidates in detail, but at the same time, it is quite challenging to work with such multi-source information. [4,5,10]

The capabilities of AI to process large sets of data and detect patterns and correlations are valuable in this context since they allow for exploring the connection between particular properties and activities of molecular structures. [5,8]

B. High Cost and Long Development Time

High costs of failed trials and the overall long duration of the drug discovery and development process make it necessary to reduce the number of experimental iterations. [1,3,4]

Researchers note that the current low efficiency of traditional pharmaceutical science stimulates the need for alternative approaches that would allow for choosing the most promising candidates and eliminating unsuccessful ones at an early stage. [3,5]

Therefore, AI's ability to predict the properties of molecular structures and screen them for desirable characteristics can be beneficial for contemporary pharmaceutical science. [2,13]

C. High Attrition of Drug Candidates

The failure of clinical candidates is commonly explained by their insufficient efficacy or unacceptable side effects, as well as pharmacokinetic properties. [1,3] Thus, the ability of AI to predict biological activity and ADMET properties is valuable in pharmaceutical research since it allows for separating unpromising candidates early in the process. [11,13]

D. Increasing Chemical Libraries

The rapid growth of chemical libraries and the increasing number of potential drug candidates stored therein are a complex challenge in modern pharmaceutical science. [14-20] Computational exploration of such databases is often the most practical way to study the properties of each molecule, which makes the use of AI technologies essential. [10,20]

IV. MAJOR APPLICATIONS OF AI IN DRUG DISCOVERY

A. Target identification and validation

Target identification is one of the initial steps of drug discovery. To be viable, a target should have a substantial link with the disease and/or be amenable to therapeutic modulation [1,3].

AI can be applied to genomics, transcriptomics, proteomics, and bioinformatics to identify disease-target linkages and connections between targets and therapeutics [15,16,19].

Such connections can be established using knowledge graphs and network approaches. These methods are particularly beneficial in cases when information from different databases needs to be combined, and relationships between diseases, genes, proteins, and targets need to be discovered [17,18].

It is essential to note that while AI can assist in target identification, it cannot replace traditional laboratory experiments. Thus, AI-driven discovery efforts should be used to triage and prioritise targets for further wet lab experiments [2,5].

B. Virtual Screening

Virtual screening generally refers to the in-silico assessment of thousands to millions of compounds to select the most promising hits for further research [20,21].

Virtual screening tools typically rely on ML algorithms which were initially trained on existing data about relationships between compounds and targets. The application of such algorithms allows for reducing a large list of potential molecules to dozens or hundreds of compounds that can then be tested in vitro or in vivo [9,13,21].

More recent developments enable the use of deep learning approaches for virtual screening. For instance, the tool Deep Docking was created as a deep learning-based platform which enables large-scale structure-based virtual screening [20].

The value of virtual screening should be seen in its ability to triage and prioritise. Thus, while computationally identified molecules may show great promise, they still need to be tested experimentally. A computational prediction cannot be used as an absolute indicator of a compound's biological activity [5,20].

C. Molecular Docking

Molecular docking is a computational technique which predicts the most likely binding modes of a ligand to a protein target. In practice, the method tries to find the optimal ligand-binding pose and uses scoring functions to rank different binding modes [21,22].

AI applications can benefit molecular docking in several ways, including optimisation of scoring functions, identification of binding site features, and ranking of molecules [20-22].

The combination of molecular docking and ML methods can substantially improve virtual screening to benefit virtual screening tremendously. However, it is crucial to remember that the results of molecular docking should be used as an indication of potential binding rather than a direct measurement of a molecule's binding affinity to a target [5,20,21].

V. AI IN QSAR AND MOLECULAR PROPERTY PREDICTION

Quantitative structure–activity relationship (QSAR) modelling typically aims to relate compound structure to a property of interest. [9,12] Traditional QSAR approaches have been widely applied in medicinal chemistry, while machine-learning methods enable modelling of more complex, non-linear relationships. [9,12,13]

AI-driven QSAR models can be used to predict biological activity based on molecular descriptors, fingerprints or other representations. [12,13] These models can help to prioritise compounds with desirable properties for synthesis or biological evaluation. [11,12]

Deep-learning approaches have also been used to predict molecular properties, by learning relationships between molecular representations and experimentally determined targets. [7,9,10]

Performance of QSAR model is typically poor when it is queried about compounds outside the scope of the training set. For this reason, careful validation and applicability domain assessment are critical for QSAR-based studies. [5,6,13]

VI. AI IN ADMET PREDICTION

ADMET is a scientific term that means Absorption, Distribution, Metabolism, Excretion and Toxicity. In general, ADMET properties are closely linked to a compound's overall success in drug discovery. [2,11]

A compound may well have desirable target engagement properties, but if it has poor ADMET properties, it will likely fail in clinical trials. [1,11]

AI-driven approaches can be used to predict a range of ADMET-related properties, including physicochemical, pharmacokinetic and toxicity characteristics. [9,11,13]

By enabling early predictions of these properties, AI can help to guide lead optimisation. This is particularly important for ADMET, since properties such as absorption or metabolism become more difficult and costly to optimise at later stages of development for clinical trials. [2,11]

It is very important to notice that ADMET prediction very much relies on the quality of the set of training data. On that conditions, computational ADMET evaluation data should be used for assessment of as an adjunct to traditional preclinical pharmacokinetic/toxicology study. [5,6,11]

VII. AI IN DE NOVO DRUG DESIGN

De novo drug design is fundamentally different from virtual screening, since it focuses on the generation of novel compounds rather than the identification of existing molecules. [23,24]

A number of AI-driven approaches have been used for de novo design, including generative models, recurrent neural networks and reinforcement learning. [23-25]

These approaches can be used to design molecules with specific properties, including biological activity, desirable physicochemical characteristics or a combination of several features. [23-25]

An AI-assisted de novo design can be broadly divided into the following stages:

Define design goals → AI-based molecule generation → *In silico* filtering → Activity/ADMET prediction → Lead optimisation → Experimental testing. [23-25]

VIII. AI IN LEAD OPTIMISATION

Lead optimisation refers to the iterative process of optimizing a hit or lead compound to improve potency, selectivity, and other pharmaceutical properties as well as safety and other desired attributes. [2,3]

AI can help in lead optimisation by analysing existing structure–activity relationships and predicting the effect of structural modifications on biological activity and physicochemical properties. [11,13]

Multi-parameter optimisation is of particular importance, as drug candidates usually need to simultaneously fulfil multiple design criteria, since a molecule that is highly potent but shows unacceptable toxicity or poor solubility, for instance, is unlikely to reach the market. [3,23] Therefore, AI can help medicinal chemists in prioritising modifications that are likely to yield the most promising results in terms of drug design. [23,25]

IX. AI IN COMPUTER-ASSISTED CHEMICAL SYNTHESIS

Beyond hit and lead generation, AI can also play a role in the downstream stages of drug discovery, such as chemical synthesis. Specifically, AI can help researchers in designing synthesis routes to produce the target molecule, based on retrosynthetic analysis. [26,27] The latter typically involves working backward from the core structure of the molecule of interest and identifying possible precursor compounds that can be used to synthesise it via specific reaction steps. Deep learning and symbolic artificial intelligence have been employed to develop automated retrosynthetic planning software. [26]

AI can support the design of organic synthetic routes through the following tasks by contributing to: [26,27]

1) Reaction prediction,
2) Retrosynthetic analysis,
3) Selection of starting materials,
4) Synthetic-route design,
5) Prediction of optimal reaction conditions.

The use of AI in this area facilitates faster evaluation of different reaction pathways and optimisation of the overall retrosynthetic plan. However, proposed synthetic routes still require expert evaluation and experimental validation. [5,26]

X. AI IN DRUG REPURPOSING

Drug repurposing typically refers to the process by which existing therapeutic agents are repositioned for the treatment of other diseases. [27-29] Compared to de novo drug discovery, drug repurposing is often associated with shorter timelines and reduced failure rates, as relevant pharmacological, toxicological, and clinical information on the therapeutically active molecule is already available. [27,29]

AI can be used for drug repurposing by computationally mining and evaluating drug–target relationships, disease ontologies, molecular networks, and other data to identify potential drug–disease associations. [28,29] Both machine learning and network-driven approaches have been employed to predict new indications for approved drugs or bioactive compounds. [28,29]

Drug repurposing became of particular interest in recent years due to the need for rapid identification of therapeutic agents for emergent infectious diseases such as COVID-19; however, computational predictions usually require extensive experimental validation in vitro and in vivo before clinical evaluation can commence. [27-29]

XI. AI IN PRACTICAL DEVELOPMENT

AI can be used for predicting pharmacological, pharmacokinetic, and toxicological properties of candidate molecules. [2,11,13]

These computational models can help researchers to prioritise molecules for further analysis and testing. [11,13]

Moreover, employing AI can help to interpret results from various experimental platforms, elucidating connections between molecular properties and their effects. [4,7]

It is noteworthy that biological processes are complex dynamic systems, meaning that experiment-based validation of computational predictions is essential. [5,6]

XII. AI IN CLINICAL TRIALS

The role of AI is not limited to molecular design and discovery, since researchers are integrating it into clinical development processes. There are several areas in which AI can be incorporated into clinical trials, including patient stratification, identification of biomarkers, trial recruitment, trial-site selection, and data analysis. [2,30-33]

For instance, machine learning models can identify patterns associated with clinical trial progression and outcomes. [30,33]

Additionally, employing AI for mining clinical data and electronic health records can support the selection of appropriate patients and optimise trial recruitment. [30,31]

Nevertheless, because there are high stakes in clinical trials, mistakes in patient stratification, data analysis, or other areas could lead to significant losses. Thus, it is essential to ensure that AI-based processes are transparent, reliable, and valid. [31-33]

XIII. AI IN PHARMACEUTICAL FORMULATION AND DRUG DEVELOPMENT

AI applications are not restricted to studying molecular properties and interactions. Researchers are integrating computational models into pharmaceutical formulation, drug design and discovery, manufacturing, and other areas. [2,34,35]

For example, AI can be utilised *in silico* formulation development, in which researchers analyse how certain formulations influence the properties of a drug. [34]

Such an approach allows investigators to optimise formulations and reduce the number of experiments needed for testing. [34,35]

Furthermore, it is possible to apply similar concepts to manufacturing, where predictive models help researchers control the process and ensure high product quality. [35]

In general, the implementation of AI in various stages of pharmaceutical development and clinical trials allows researchers to innovate and optimise multiple areas at once. [2,34,35]

XIV. ADVANTAGES OF USING AI IN DRUG DISCOVERY AND DEVELOPMENT

There are several advantages of using AI in pharmaceutical research and development. First, it enables faster analysis of large data sets, helping researchers identify valuable patterns researchers to find valuable patterns. [4,5]

Second, by employing AI in virtual screening and compound prioritization, it becomes possible to reduce the number of compounds under consideration. [20,21]

Third, QSAR and related models can predict ADMET properties and toxicity profiles ADMET properties and toxicity profiles, which reduces the number of experiments needed for assessing these aspects. [11-13]

Fourth, using generative models and optimisation algorithms can facilitate molecular design by helping researchers identify molecules with desirable properties. [23-25]

Fifth, AI can also be utilised in retrosynthetic chemistry to find potential pathways for synthesizing target molecules. [26]
Sixth, AI can be leveraged for drug repurposing for drug repurposing by integrating biomedical information and identifying molecules with new applications. [28,29]
Finally, in clinical development, employing AI supports decision-making and optimises trials. [30-33]
Overall, the main advantage of using AI in pharmaceutical research is that it helps to optimise decision-making and prioritise high-yield options. [1,2,4]

XV. CHALLENGES AND LIMITATIONS

A. *Data Quality*

The quality of data used to train an AI system significantly impacts its performance. Inaccurate, insufficient, erroneous, or biased data may lead to low prediction accuracy or erroneous findings. [5,6,10]

B. *Data Scarcity*

Pharmaceutical research poses significant challenges to conventional ML due to the limited number of experimentally validated instances. This is especially true for complex multi-layer ML systems, which require extensive training data sets to function correctly. [5,6]
Modern ML approaches to pharmaceutical research include transfer learning, multi-task, active, and other techniques that aim to maximize the amount of information obtained from a small set of training samples. [11,23]

C. *Overfitting*

An ML model may perform well on training-like data but poorly on unseen or out-of-distribution data. [5,6].
Therefore, proper train-test partitioning, validation procedures, and, where possible, external validation of ML models are essential. [13,36-38]

D. *Black-Box Problem*

One of the significant challenges posed by complex ML systems is their black-box nature. In other words, complex ML models may provide limited interpretable rationale for their predictions its decision-making process. [28,37]
This limitation is especially challenging when working with pharmaceutical data, as most researchers need to understand the biological rationale behind the predictions made by an ML model. [28]
Another approach is to develop more interpretable AI systems capable of providing adequate explanations for their actions. This direction is especially relevant for computational drug discovery, where Explainable AI is a major research priority. [28]

E. *Chemical-Space Limitations*

The performance of an ML model is primarily determined by the composition of the data set used to train it. More specifically, it is critical to use data similar to the type of compounds for which an ML model is intended. [5,6,13]

F. *Regulatory Concerns*

The use of AI in pharmaceutical research raises critical regulatory issues, including data provenance, methodological validation, reproducibility, and transparency. [31,36,37]
These issues are especially acute in pharmaceutical research because AI-driven approaches have the potential to impact decision-making in drug development significantly. [31,36]

G. *Lack of Multidisciplinary Expertise*

The field of AI pharmaceutical research is multidisciplinary by nature, thus requiring a team of researchers with different specializations. Notably, a team of scientists working on pharmaceutical AI applications should consist of people with expertise in pharmaceutical studies, statistics, data science, and biology. [1,2,4] Therefore, the lack of expertise in any of these areas may impede progress in AI-driven pharmaceutical research. [4,5]

XVI. ETHICAL AND REGULATORY CONSIDERATIONS

AI-driven pharmaceutical research involves numerous ethical and regulatory challenges stemming primarily from the volume of information such systems handle. In particular, such systems raise concerns of data privacy, governance, algorithmic bias, and responsibility. [28,31,36]

In other words, pharmaceutical research using AI requires greater levels of verifiability and accountability to ensure that the data privacy rights of the participants are not infringed and that no biases were integrated into the system design. [28,31,33]

Another critical consideration pertains to the reproducibility of results. An ML model is only as good as the data set it was trained on. [5,6,37] To ensure reproducibility, it is essential to report all details about the data set, including information about how it was compiled, processed, and utilised to train the ML model. [37-40]

Finally, it is essential to recognize that future regulatory policies concerning the use of AI in pharmaceutical research must promote a balance innovation with drug quality, efficacy, and patient safety drug quality, efficacy, and patient safety. [31,36]

XVII. CONCLUSION

Artificial intelligence is becoming an essential part of the drug discovery and development process. Its role now extends from target discovery and virtual screening to QSAR modelling, ADMET prediction, de novo design, lead optimisation, synthesis planning, drug repositioning, and clinical development.

The most significant advantage of AI lies in its ability to analyse extensive and multidimensional data sets while helping to make decisions based on the information. By prioritizing hits and predicting valuable properties, AI-driven technologies can help reduce trial-and-error through better prioritisation of candidates in pharmaceutical research while accelerating progression through the drug development pipeline.

At the same time, one should not forget that AI is only a tool. The issues of data quality, insufficient training sets, overfitting, interpretability, and external validation limit its capacity to achieve better results. The most plausible scenario suggests that AI will not replace medicinal chemists, pharmacologists, biologists, and clinicians in the drug-discovery process but rather complement them, benefiting from cross-disciplinary collaboration. Thus, the implementation of artificial intelligence in pharmaceutical research and development will ultimately depend on how wisely the experts in the field can utilise these opportunities.

CONFLICT OF INTEREST: None

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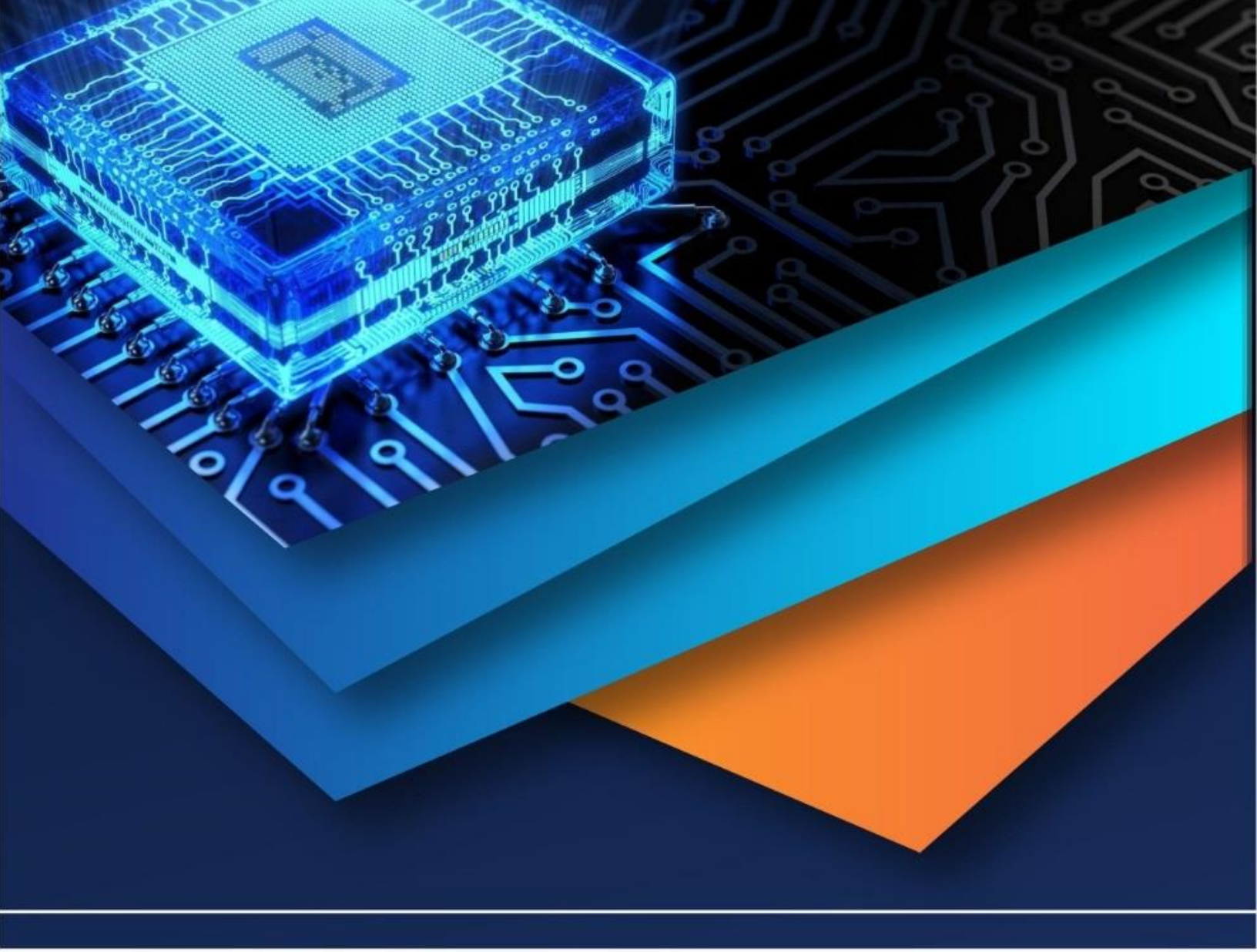

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