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A REVIEW ON ARTIFICIAL INTELLIGENCE MACHINE LEARNING IN DRUG DESIGN

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ABSTRACT

The global spread of COVID-19 has raised the importance of pharmaceutical drug development as intractable and hot research. Developing new drug molecules to overcome any disease is a costly and lengthy process, but the process continues uninterrupted. The critical point to consider the drug design is to use the available data resources and to find new and novel leads. Once the drug target is identified, several interdisciplinary areas work together with artificial intelligence (AI) and machine learning (ML) methods to get enriched drugs. These AI and ML methods are applied in every step of the computer-aided drug design, and integrating these AI and ML methods results in a high success rate of hit compounds. In addition, this AI and ML integration with high-dimension data and its powerful capacity have taken a step forward. Clinical trials output prediction through the AI/ML integrated models could further decrease the clinical trials cost by also improving the success rate. Through this review, we discuss the backend of AI and ML methods in supporting the computer-aided drug design, along with its challenge and opportunity for the pharmaceutical industry

KEYWORDS: *Artificial intelligence, Machine learning, Deep learning, Pharmaceutical industry, Imaging*

I. INTRODUCTION

The global spread of COVID-19 has raised the importance of pharmaceutical drug development as intractable and hot research. Developing new drug molecules to overcome any disease is a costly and lengthy process, but the process continues uninterrupted. The critical point to consider the drug design is to use the available data resources and to find new and novel leads. Once the drug target is identified, several interdisciplinary areas work together with artificial intelligence (AI) and machine learning (ML) methods to get enriched drugs. These AI and ML methods are applied in every step of the computer-aided drug design, and integrating these AI and ML methods results in a high success rate of hit compounds. In addition, this AI and ML integration with high-dimension data and its powerful capacity have taken a step forward. Clinical trials output prediction through the AI/ML integrated models could further decrease the clinical trials cost by also improving the success rate. Through this review, we discuss the backend of AI and ML methods in supporting the computer-aided drug design, along with its challenge and opportunity for the pharmaceutical industry.

The global spread of COVID-19 has raised the importance of pharmaceutical drug development as intractable and hot research. Developing new drug molecules to overcome any disease is a costly and lengthy process, but the process continues uninterrupted. The critical point to consider the drug design is to use the available data resources and to find new and novel leads. Once the drug target is identified, several interdisciplinary areas work together with artificial intelligence (AI) and machine learning (ML) methods to get enriched drugs. These AI and ML methods are applied in every step of the computer-aided drug design, [1]

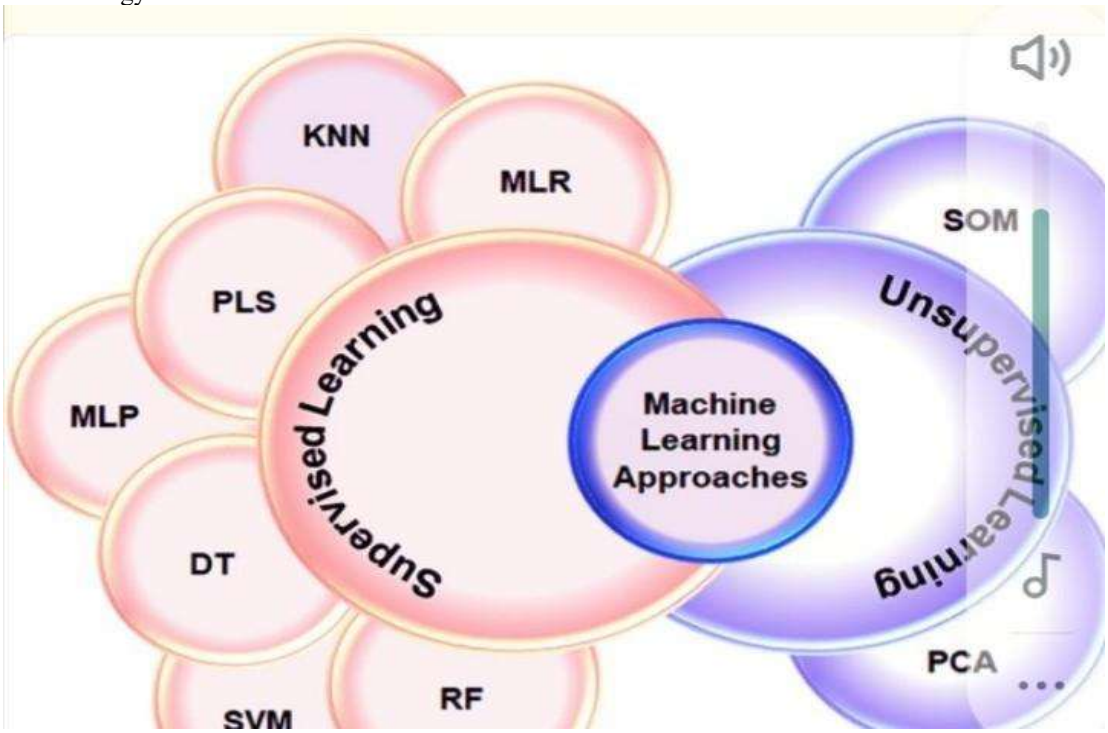
The ground-breaking development in biomedical research has shown an increase in the availability of biomedical data But researchers have raised whether the transmission and transfer of biomedical data are done correctly to extract practical knowledge . Especially in the pharmaceutical sector, there have been several pieces of research, research outcomes, clinical data, and ethnic population-wise data, and other experimental data are available. In this case, the pharmaceutical sector with drug discovery is a process that is very costly, time-consuming, and subject to many formalities. The average cost for getting a new drug by the various phase of drug development can range from $1 to $2 billion and consumes up to 15 years .Upon considering the research question, the available data on this domain can be used to develop new drugs, which can be more accurate, timely, and cost-effective.Researchers worldwide are continuously developing

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innovative methods and algorithms to obtain suitable molecules with a short time and cost-effectiveness. Significantly, the introduction of artificial intelligence (AI), deep learning (DL), machine learning (ML), and computational chemistry towards drug discovery has shown a significant impact on its success rate. These methods alone or jointly combine to form new strategies that incorporate a wide range of efficient algorithms that enhance the predictions.[2]

Computation power and algorithms for developing new leads with therapeutic importance in the modern drug designing process play a vital role. This current technological era is showing the technical update regularly . Nowadays, several types of research offer deep atomic insights, which tend to establish the cause of disease, function, or inhibitions. Based on that, the algorithms are also updated to respond to the atom's realistic mechanistic action that is core important for the drug designing process. For the Computer-Aided Drug Designing (CADD), the designing process initiates with two methods. One approach is structure-based drug design (SBDD), and the other one is ligand-based drug design (LBDD). But both ways heavily rely on the backend algorithms, scoring functions, and force fields for ranking and evaluating the energy contribution of lead molecules in the molecular systems. As of now, there have been many programmes or software applications that run with various algorithms, interpreting the results with predefined scoring functions for both SBDD and LBDD methods. But predicting the exact parameterization and obtaining the accurate energy levels and transferable force fields are challenging tasks for filtering the possible drug molecules . To solve those issues, the parameterization process with the input of quantum physics of significant dimensions with a small number of parameters and a simple, functional analytic form is also introduced. In this way, the CADD and molecular modelling approaches enhance the efficiency of predicting the lead molecules by lowering the error components. The specialty of CADD and molecular modelling drives many small molecules or whole small molecules databases in a limited time and can show realistic interactions between the hit molecules and macromolecules. Macromolecules are composed of polymeric units of amino acids or nucleic acids and the predefined algorithms. The force fields are programmed to adjust these atoms in these macromolecules. There are several programmes, software applications, and web servers available, but the user must choose the backend algorithm and force fields according to the macromolecules of their requirements.

Tha Introduction of modern AI methods offers highly reliable computational methods in pharmaceutics and biomedical science. AI simulates human intelligence to machine models to rehabilitate or imitate human performance. Specifically, the MI approach can correct complex chemical problems in the drug identification process. This field of interest is not limited to certain areas, as every domai applies the automation traits in link with human minds for thinking, learning, and problem-solving efficiency.



. **Fig:1**

The integration of AI and ML into biomedical applications is shown in Fig. 1. It clearly shows the AI and ML with computational advances and statistical methods are incorporated into biomedical applications to mimic human thinking, reasoning, and implementation [15].momentum with huge success by providing novel drug

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II. E ARTIFICIAL NEURAL NETWORKS

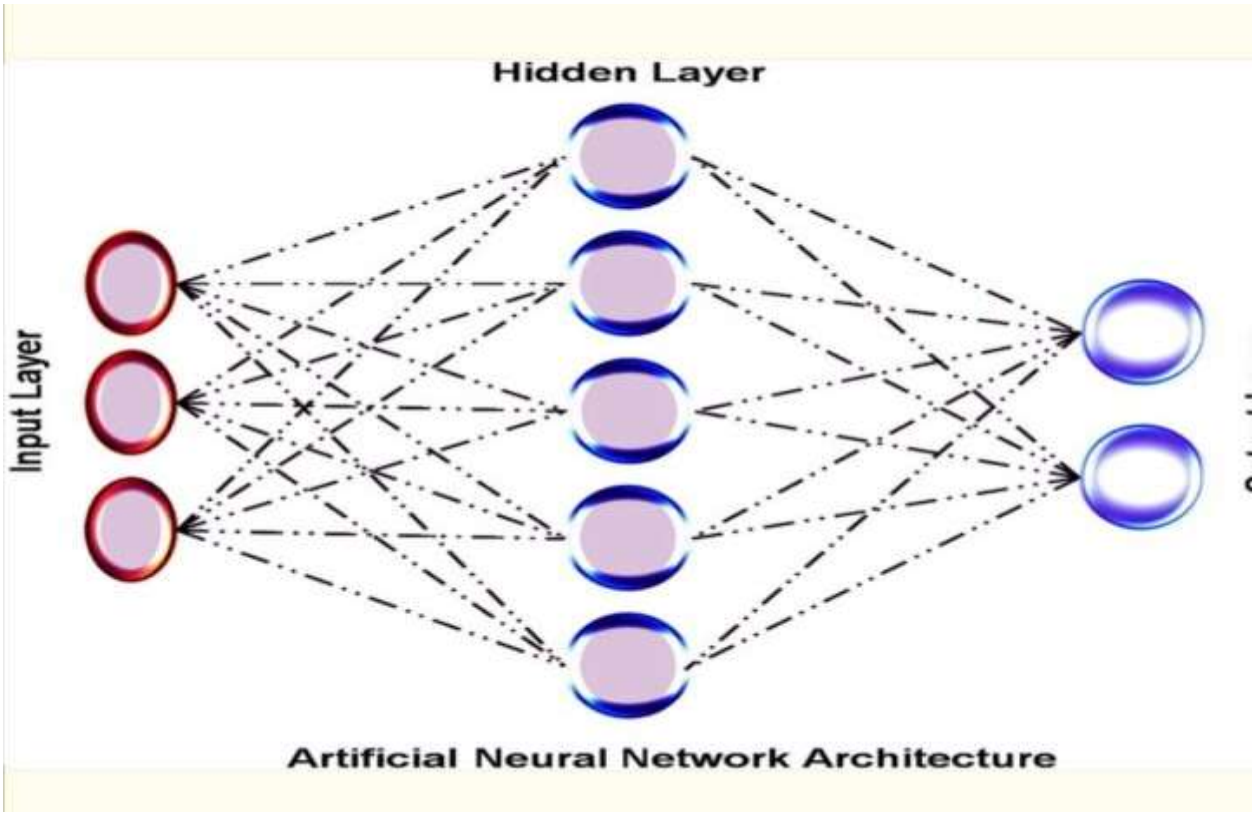


Fig:2

Artificial neural networks (ANNs) are favourably recognized computer models developed based on the Homo sapiens brain and its networking trends . The simplest case shows a fully connected network or feed-forward that shapes the computation chart with three layers (input layer, hidden layer, and output layer. The layer-wise single computing unit called neurons works as a nonlinear transformation to the input data. This information is propagated in layer-wise mode and receives the output of the preceding layer as shown in Molecular modelling and drug design predominantly rely on ANNs. It resolves the complexity associated with statistical models used in HTVS (high-throughput virtual screening), QSAR (quantitative structure–activity relationship), and pharmacokinetics and pharmacodynamics studies. For the numerical values determining the output, ANNs perform excellently in interpreting nonlinear relationships and predict the process of success in the drug finding process.[3]

Basic model of artificial neural network architecture proposed where the input layer is modelled for network inputs, output layer is modelled for network outputs, and in between the hidden layer is modelled for the feed-forward and back-propagation function[4]

III. APPLICATION OF ARTIFICIAL NEURAL NETWORKS IN DRUG DISCOVERY

As discussed above, ANNs have high reliability towards improving efficiency and target-based drug discovery. It has a massive ability towards complex investigation and nonlinear relationships, and so this ANN is alternatively called “Digitalized Model Brains”. Neural network (NN) applications are highly accountable for STEM (Science, Technology, Engineering and Medicine). Especially in the molecular modelling and pharmaceutical sciences, the ANNs’ application sets the trend by providing high reliability of results . Notably, the ANNs used to scrutinize the extensive database of small molecules (HTVS), property prediction (ADME/T), QSAR, pharmacophore analysis, pose validation, formulation and development of leads are shown in F [5]

IV. CONCLUSION

In summary, many factors impact the successful integration of AI and machine learning into drug discovery and development and the pharmaceutical industry for ploy pharmacology, drug design, drug screening and drug repurposing. Advances in technology, including those based on AI, will always be required to reduce the time and money spent on research, development and production, and to increase efficiency.

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This systematic literature review showed that AI and machine learning can improve the efficiency and accuracy of drug discovery and development. These technologies not only augment process efficiency, but also in some cases reduce or eliminate the need for clinical trials by conducting simulations in their place, and also allow researchers to study molecules more extensively without trials, reducing costs as well as ethical concerns. Integrating AI and machine learning is likely to revolutionise drug development in time, but there are still a number of barriers like cleaning of unstructured and heterogeneous dataset, occasional incompetency of the computing device etc.

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