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Review Article

The Revolutionary Role of Artificial Intelligence (AI) in Pharmaceutical Sciences

Amaresh Prusty*, Susanta Kumar Panda

Department of Pharmaceutics, Royal College of Pharmacy and Health Sciences, Berhampur, Odisha, INDIA.

ABSTRACT

The traditional drug discovery process is expensive, time-consuming, and often leads to a high failure rate. The development of numerous new medications in the pharmaceutical sciences is only one example of how the advancement of artificial intelligence has opened up exciting new opportunities for developing intelligent modelling. Machine learning and deep learning are two examples of artificial intelligence that can sift through large datasets in search of promising new drugs. AI algorithms can predict the binding affinity of molecules to specific targets, helping researchers narrow down the pool of potential drug candidates. Pharmacokinetics and pharmacodynamic are essential aspects of drug development. Drug formulation development requires extensive testing and optimization of various parameters. AI models can quickly analyze data from multiple experiments and identify the most promising formulations, saving time and resources. New pharmaceuticals may be developed and brought to market at a reduced cost and in a shorter amount of time with the use of AI-based optimisation approaches. Absorption, Distribution, Metabolism, and Excretion (ADME) are only some of the aspects of pharmacological physiology that may be modelled and predicted with the use of artificial intelligence. By integrating AI models into the drug development process, researchers can gain a deeper understanding of a drug's pharmacokinetic and pharmacodynamic properties. This knowledge helps in designing drugs with improved efficacy and reduced side effects. So, in present topic authors tried to give insights how AI is playing a transformative role in pharmaceutical sciences. As AI technology continues to advance, the future of pharmaceutical sciences looks brighter than ever.

Keywords: Machine learning, Artificial intelligence, Drug discovery, Target identification, Artificial Neural Network (ANN).

Correspondence:
Dr. Amaresh Prusty
Department of Pharmaceutics, Royal College of Pharmacy and Health Sciences, Berhampur-760002, Odisha, INDIA.
Email: amareshprusty@gmail.com

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INTRODUCTION

The research and development of new medications is a costly and time-consuming endeavour. Research in pharmaceutical sciences and the development of novel compounds has been hindered in recent years by a lack of cutting-edge methods.[1,2]

The main goal of drug development is to find medicines that can help to avoid or treat certain illnesses. Many pharmaceuticals are small, chemically synthesised compounds with the ability to bind to and inhibit the activity of certain disease-related molecules (often proteins). To find promising compounds with the potential to become medications, researchers often run extensive screenings of libraries or many rounds of experiments, which is not only costly but also time-consuming. Pharmaceutical research is a high-risk, high-cost enterprise with substantial effects on human health and the pharmaceutical industry; the latest estimates put the cost of bringing a new medicine to market at roughly US $2.6 billion.[3] The pharmaceutical research process for discovering and developing new drugs is intricate and challenging, encompassing high risks and substantial costs. The pharmaceutical industry is very responsive to these issues because of the profound effects they have on numerous facets of human health. Significant efficiency improvements within the area of drug research and development are needed to overcome these problems and minimise cycle time and cost.[4,5] Despite the potential shown during laboratory testing, a new drug candidate may still face failure in clinical trials. This is evidenced by the fact that less than 10% of drug candidates successfully reach the market following Phase I trials. Numerous therapeutic compounds may be developed because to the enormous chemical space that is available. However, due to a dearth of cutting-edge technology, the medication development process is both lengthy and costly. Artificial Intelligence (AI) has developed as a useful tool for analysing large and complicated data sets in order to circumvent these constraints. By leveraging AI, researchers can accelerate the drug discovery process and reduce costs significantly. AI's potential in drug discovery holds

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promise for transforming the pharmaceutical industry's future and addressing current challenges effectively.[6-11] Hit and lead compounds may be identified with the use of AI, and the findings can be verified by the determination of the drug's target.[12,13] AI has emerged as a major tool for analysing voluminous and high-dimensional data in pharmaceutical research, helping to overcome previous barriers to medication discovery. Researchers want to quicken the pace of drug development and lower associated expenses by tapping into AI systems' unrivaled data processing capability. According to Bekryl, a market research organisation, the application of AI in pharmaceutical research might save more than US $70 billion in drug development costs by 2028. By relying on chemists to develop, synthesize, and analyse a large number of compounds without first subjecting them to a broad screening process, rational structure-based drug discovery techniques are gaining popularity.

Reasoning, knowledge representation, and problem-solving are only few of the many methodological areas that make up AI. Machine learning (ML) is a central paradigm in artificial intelligence that makes use of algorithms to discover regularities in data. As a subsection of ML, Deep Learning (DL) uses ANNs to simulate the way neurons in the human brain communicate with one another. ANN can be trained using supervised or unsupervised methods, and they come in a variety of forms such as Multilayer Preceptor (MLP) networks, Recurrent Neural Networks (RNNs), and Convolution Neural Networks (CNNs).[14-17] Drug discovery, dosage form development, optimization, and pharmacokinetic and pharmacodynamic research all benefit from the use of AI. Prior information collected using various domains, such as Pub Chem, Chem Bank, Drug Bank, and Chem DB, can help in showing bioactivity and selecting potential drug candidates. Virtual screening using in silico approaches allows for more serious examination, faster removal, and more comprehensive collection of substances. When choosing a lead compound with the appropriate activity, AI-driven algorithms take into account their physical, chemical, and toxicological properties.[18-21] Algorithms used in drug development now take into account a substance's physical, chemical, and toxicological properties when choosing a lead compound to bind with and create activities. The efficacy and biological activity may be enhanced by a variety of physicochemical properties.[22,23]

Artificial intelligence-based Quantitative Structure-Activity Relationship (QSAR) models are used to predict physicochemical qualities like lipophilicity and solubility. These forecasts have been made using DL and ANN models trained using the ADMET predictor and the ALGOPS software. New chemical entities may be predicted with the use of these models, which take into account factors like surface area, mass, hydrogen count, refractivity, volume, log P, and solubility index.[24-27] In order to predict the binding characteristics of molecules, algorithms use molecular descriptors like Simplified Molecular Input Line Entry System (SMILES).[28] The different physicochemical parameters are often determined using a Quantitative Structure-Property Relationship (QSPR) known as the Estimation Program Interface Suite.[29] AI-driven virtual screening of compounds from vast chemical spaces, such as PubChem, Chem Bank, Drug Bank, and Chem DB, aids in selecting appropriate molecules for further testing. Efficient profile analysis, rapid removal of non-lead compounds, and molecule selection are all made possible with the use of structure and ligand-based methodologies, as well as in silico technologies. Through the use of big data modelling and analysis, AI also plays an important part in determining whether or not a certain medication molecule is safe and effective for human use. In ADMET data sets of drug candidates, deep learning models have shown superior predictivity compared to classical ML techniques.[30-32] To investigate the potential benefits of DL in the pharmaceutical industry's drug development process, Merck hosted a QSAR ML competition in 2012. When comparing DL and classic ML methods for assessing ADMET (absorption, distribution, metabolism, excretion, and toxicity) data sets of drug candidates, the DL models showed exceptional predictivity.[33-35] Molecules that seem promising for future testing may be chosen with the use of Virtual Screening (VS) in numerous open-access chemical spaces including Pub Chem, Chem Bank, Drug Bank, and Chem DB. Improved profile analysis, quicker removal of non-lead compounds, and identification of candidate therapeutic molecules are all made possible by the use of in silico methodologies in addition to structure and ligand-based approaches, which leads to cost savings.

The physical, chemical, and toxicological properties of a drug's target molecules are carefully considered by drug design techniques like Coulomb matrices and molecular fingerprint identification. The intended chemical structure of a drug may be accurately predicted using a mix of prediction models, molecular similarity evaluation, molecule creation procedures, and in silico methodologies.[36] For the docking of 40 receptors and 2950 ligands, Pereira et al. proposed a novel approach dubbed DeepVS. When tested against 95,000 decoys, this approach performed very well on these receptors.[37] In addition, the form similarity, pharmacological activity, and physicochemical features of a cyclin-dependent kinase-2 inhibitor were optimised using a multi-objective automated replacement approach.[38] QSAR modelling techniques have advanced into AI-based methodologies such as Linear Discriminate Analysis (LDA), Support Vector Machines (SVMs), Random Forest (RF), and decision trees, allowing for quicker QSAR research and the discovery of possible medication candidates. These AI developments may completely change the drug discovery process by allowing for faster and more precise candidate for drug identification.[39,40]

AI's vast potential in analyzing data, predicting properties, and optimizing drug design holds immense promise for the pharmaceutical industry's future. With continued advancements

in AI technology, the efficiency and effectiveness of drug development are expected to improve, leading to better patient outcomes and advancements in medical science.

Basic concepts of AI and its scope of application

AI has a long history, dating back to its proposal at the Dartmouth Conference in 1956. It was described at the time as an algorithm that gives robots the capacity to think for themselves and carry out numerous tasks. SVM and ANN are two examples of the cutting-edge technology that have emerged as a result of AI's development from its perceptual machine roots. Despite facing some challenges and setbacks, AI has seen significant progress, particularly due to the availability of advanced hardware support.

In the realm of computer science, AI is considered a branch that focuses on problem-solving using symbolic programming. It has the potential to revolutionize various industries, including pharmacy. A considerable amount of research is being conducted to enhance the current AI technology, aiming to make the pharmacy profession more efficient and effective by discovering the new drug molecule along with its formulation and optimization parameters. The integration of AI in pharmaceutical research and development can lead to significant advancements and streamlined processes, ultimately benefiting patient care and the healthcare industry as a whole.[41] In a broader senses the main components of AI are Deep learning, Machine learning, Computer vision, Cognitive computing and Artificial neural network.

Machine learning has a branch called deep learning. The human brain's biological neural networks serve as inspiration for these artificial neural networks, which are designed to function similarly to the way those neurons in the brain process data. They are capable of determining a single output from multiple inputs by using multiple layers of networks that work together. Positive and negative reinforcement are used in the learning process of deep learning, which needs continuous processing and reinforcement to make progress. One area where deep learning has been put to use is in automatic voice identification and translation. It can also be applied in manufacturing processes, such as drug formulation and monitoring, to streamline operations and reduce human intervention.

Machine learning, on the other hand, is a more general use of AI that relies on specially programmed computers to do a variety of tasks. Without the need for manual coding, it enables systems to automatically learn and improve as they go along. Healthcare, pharmacology, and the biological sciences are just a few of the many fields that might benefit from machine learning. In the pharmaceutical industry, machine learning is used for tasks such as grinding, mixing, granulating, drying, filling, packing, and testing. It is also widely used in analytical testing, such as High-Performance Liquid Chromatography (HPLC), High Performance Thin Layer Liquid Chromatography HPTLC, Nuclear Magnetic Resonance (NMR), Differential Scanning Calorimetry (DSC), and Thermo Gravimetric Analysis (TGA). Moreover, machine learning is employed in genetic data sequencing, coding, and data recognition to develop biomedicines. Graphs, tables, photographs, and other text and video may all be understood with the help of computer vision, a branch of AI that use deep learning and pattern recognition to decipher the information contained inside PDF documents which is utilised to speed up patient diagnoses by analysing X-rays. Computer vision is also applied to identify chemical components, formulate complexation, and analyze genetic structures.

Cognitive computing is another aspect that aims to recreate the human thought process in a computer model. The goal of cognitive computing is to simulate human reasoning in a digital environment. Human language and the interpretation of visuals are essential to this. Coupling human-like behaviour with advanced computational and information processing capabilities, this is the goal of cognitive computing and artificial intelligence. Teaching robots to comprehend human language in context and respond sensibly is meant to pave the way for frictionless interactions between people and technology.

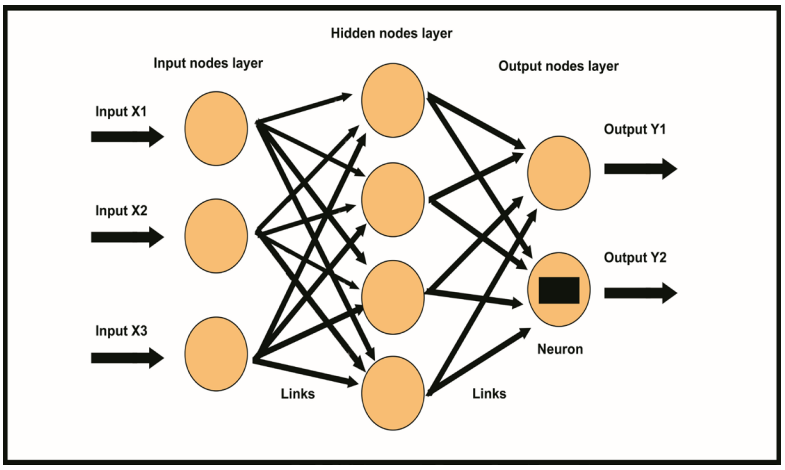

Figure 1: Basic of artificial neural network.

Artificial neural network model involves computations and mathematics, which simulate the human–brain processes as shown in Figure 1. By combining experimental and evidence-based data during drug discovery, ANN is able to tackle complex difficulties in the drug discovery process by absorbing information and drawing meaningful conclusions from Quantitative structure-activity relationship, Quantitative Structure-Toxicity Relationship (QSTR), pharmacokinetics, and pharmacodynamic studies, docking, formulation development, design of chemical synthesis, and High-Throughput Screening (HTS) study.

Different role of AI in pharmaceutical science

AI role in pharmaceutical sciences include a wide variety of academic fields that work together in the discovery, development and manufacturing of drug products.

In the Development of Drug Delivery Systems

Increased R&D expenses and decreased efficiency are presenting problems for the pharmaceutical sector in the area of medication development. However, breakthroughs in AI technology and significant increases in computer capacity have the potential to completely revamp the pharmaceutical industry. Artificial intelligence subset known as "machine learning" makes use of statistical approaches to learn automatically or via guided instruction. The use of AI tools across the medication delivery process, from initial drug development to stimulating, predicting, programming, and optimising drug distribution in patients, has the potential to greatly enhance the treatment process. Recently, artificial neural networks and other machine learning and deep learning techniques have been used to automate and improve medication development processes and distribution networks. Predicting and manipulating drug release features including solubility, rate, timing, and diffusion at sick locations is possible using ANNs-controlled drug delivery materials or devices. Drug interactions with desired targets including cellular membranes and molecular targets may also be evaluated using ANN methods. Other uses for ANN software include keeping tabs on drug encapsulation and implanting microchips with medication molecules on them.[42,43]

Advanced artificial intelligence methods have been implemented to atomize and optimize drug delivery procedures in micro particle-based drug delivery. Deep artificial neural networks and Bayesian regularised artificial neural networks have mostly supplanted older approaches like multiple linear regression and multilayer perceptron. The adoption of these newer AI methods has resulted in a faster and more cost-effective drug development process.[44] Similarly in the formulation of nano-based drug delivery system AI has an important role. The convergence of nanoscience, nanotechnology, and AI is becoming increasingly evident, given the vast amount of data at the big data level. With the help of AI and its subsystems, machine learning, and deep learning, this convergence allows improved data analytics and data mining. AI's processing capability is essential for analysing data sets that include both structured and unstructured components, such as ASCII flat files, CSV, Microsoft Excel spreadsheets, and image processing. Artificial intelligence plays a crucial part in nanomedicine, which includes cancer cells, biomedicine, and nano biology. Treatment results may be improved, and medication selection and dose determination can be accomplished concurrently thanks to AI/ML and DL platforms. Nanomedicine relies heavily on these features since diverse treatments may be included into nanocarriers, and various types of nanocarriers can be given to patients with different diseases. As a result, it is clear that the pharmaceutical sector stands to benefit much from the integration of AI, especially in the areas of drug discovery and administration. The convergence of AI with nanoscience and nanotechnology holds immense potential and opens new avenues for the field of nanomedicine.[45]

In Computer Simulation Model for ADME Study

The modern age has been ushered in by technological advancements, and technology-driven discovery has become an integral part of increasing R&D productivity and designing novel chemical entities, such as drug candidates, for use against a wide range of biological targets. Drug candidate failures in the latter phases of drug discovery and development have recently been linked to pharmacokinetic features, often known as ADME. ADME models and AI-driven computer simulations, of differing degrees of sophistication, have been created to solve this problem and aid in the screening of enormous datasets of chemicals. These models have produced tools that are more efficient than conventional methods in terms of speed, simplicity, and cost. Drug pharmacokinetics and pharmacodynamic are studied with the use of computer simulation. A drug's Pharmacokinetics (PK) refers to how it moves through your system and how it's used, while its Pharmacodynamic (PD) examines how your body responds to the medicine.[46-50] Pharmacokinetics (PK) and Pharmacodynamic (PD) are fundamental aspects of drug development and clinical practice in pharmacology. The interaction between these two disciplines plays a crucial role in determining drug efficacy and safety. Over the years, computer simulation has emerged as an essential tool in understanding and optimizing drug behaviour, enabling researchers and clinicians to make informed decisions and design effective treatment regimens. So, we may say AI based Computer simulations are used to optimize drug dosing for individual patients, taking into account factors such as age, weight, and renal function. This personalized approach improves drug efficacy and minimizes the risk of adverse effects. Simulation can predict drug concentration-time profiles based on patient data, facilitating therapeutic drug monitoring. By adjusting doses according to the predicted response, clinicians can maintain drug levels within the therapeutic window. Generally, there are mainly 4 level of the

simulations of pharmacokinetics and pharmacodynamic. In Level 1, Computer Simulation of the Whole Organism, two approaches for simulation of whole organism used and these are PK/PD model and PBPK model. The PK/PD model and the PBPK model are two methods for simulating the effects of a drug on a whole organism. The exposure-response connection is modelled using the PK/PD (Pharmacokinetic and Pharmacodynamic) model. A linear model, an E max model, or a Sigmoid E max model may be used to characterise this model, which is paired with a model of a sick state. This model is used to gather in vitro physiological and in vivo pharmacokinetic data for use in developing a PK/PD research protocol. Pharmacokinetics and pharmacodynamic serve as landmarks on the journey from exposure to reaction. A Physiology-Based Pharmacokinetic (PBPK) model is used to estimate the ADME of a synthetic or natural chemical substance in a person using a multi-compartmental model that accounts for the effects of blood and lymph flow. Many physiological organs of the body are represented in this model by separate compartments connected by the circulatory blood stream.

Similarly in Level 2, Computer simulations of isolated tissue and organ, Heart, kidney, brain; liver can be a subject of mathematical modelling research which can be carried out with distributed blood tissue model that is known as BTEX model. This is the first ever research on the biodegradation of BTEX (Benzene, Toluene, and Xylene isomer). Benzene, Toluene, and an ortho, meta, or para Xylene derivative make up the new BTEX model. The competitive inhibition, toxicity, and creation of the hazardous intermediate underlie this synergistic and/or antagonistic interaction during biodegradation of the BTEX molecule. The third level is simulation of cell, which is mainly used in biomedical research. Using an online respiratory model, researchers have created a computer simulation of a full cell and made it accessible to their user network. The Cell ML website also provides an online respiratory of the biophysical model. The directed network may be easily implemented on a computer, making it a straightforward method for modelling the intricate interaction between cells or even inside the intracellular milieu. Finally, the level 4 includes simulation of protein and genes and the goal of this method was to use an ordinary differential equation to map genetic information onto a network, with the hope of identifying the gene(s) responsible for a disease's susceptibility. Clinical data provided significant insight into the underlying disease process, allowing researchers to use simulation to pharmacology in the area of HIV/AIDS treatment creating a novel gene sequence may aid in the protein identification, translation, and transcription.

In Quality Profiling and Optimization of Drug Products

With advancements in technology and the development of modern production tools, the industry has seen improvements in quality and cost reduction due to vast research, technological developments and the introduction of innovative manufacturing gear. In pharmaceutical research Quality by Design (QbD) is gaining popularity as a method for developing products that prioritises scientific rigour and quality risk management in its emphasis on knowing both the product and the process. Quality by Design is a concept first outlined by Joseph M. Juran. Identifying hazards and providing high-quality goods depend on following the ICH Q 8 and Q 9 recommendations. Design of Experiment (DoE), a systematic way to run experiments to generate maximum output that can be carried out using tools like Minitab, Statease, and Statistica, is a crucial part of QbD. There are two approaches to experimental design. DoE is used in the screening and optimising different phases of formulation development. Screening is used to uncover important characteristics among many candidates with a minimum of experimentation. The primary goal of both the Placket-Burman and the fractional factorial design is to single out the most important effects. However, in optimisation, complete factorial designs, surface response techniques (such as Central composite, Box-Behnken), and mixed designs are often regarded to be carried out. These designing experiments are used only when certain aspects that appear to be contributing in process or formulation have been identified. During QbD approach for optimization study of different parameters are essential. Generally, the various aspects of AI which are used in pharmaceutical research (formulations) are QbD & DoE which is used to confirm the quality profile of drug product, reduce interactions among the input variables for the optimization. Based on these AI principles Prusty *et al*., developed Benidipine Hydrochloride Extended-release Matrix Tablet, by application of the Box-Behnken Design Response Surface Methodology to Study optimized formulation variables on the drug release pattern.[51] The tablets were statistically analyzed by one-way ANOVA and the quadratic response surface methodology helps in predicting the optimum levels of these factors for extending drug release. The *in vitro* drug release data were evaluated kinetically using various mathematical models based on.

Some of the important parameters which can be studied by use of AI are;

Target Product Profile (TPP) and Quality Target Product Profile (QTPP)

It reveals the high standards of the drug's quality that guarantee its effectiveness and safety. The ideal product profile will contain information on the following features: dosage form, route of administration, dose strength, pharmacokinetics, and stability. The TPP is a patient- and labelling centred concept since it highlights the product's intended performance qualities in relation to the patient's demand and is structured in accordance with the drug's most important sections of labelling. Similarly, QTPP provides a numerical alternative to concerns related to scientific security. Only patient-related efficacy that may be utilised to create and optimise a formulation and manufacturing process should be included in the QTPP. Labelling concerns

of QTPP include "identity," "assay," "dosage form," "purity," and "stability." Identity, assay, content uniformity, degradation products, residual solvents, drug release, moisture content, and microbiological limitations are all examples of quality features that might be present in a pharmaceutical product.

Critical Quality Attributes (CQAs) and Critical Material Attributes (CMAs)

CQAs are qualities (physical, chemical, biological, or microbiological) that should fall within acceptable ranges to ensure the product meets quality standards. CMAs are characteristics of raw materials that must remain within predetermined parameters in order to produce consistent, high-quality drug compounds, excipients, or intermediates.

Critical Process Parameters (CPP)

These characteristics are production process variables that may affect finished product CQAs. To determine CMAs and process parameters, risk assessment is performed throughout the product lifecycle. The Design Space is the set of input variables and process parameters that have been shown to guarantee quality.

Design Space

A pharmaceutical's Design Space (DS) is the variety of potential material and process circumstances that nevertheless guarantees high quality. This is the proven, multi-factor combination of input factors (such as material qualities) and process parameters that ensures quality.

Failure Mode Effects Analysis (FMEA)

Risk may be assessed by analysing the likelihood functions of the severity, incidence, and detectability of any event using a technique called Failure Mode and Effect Analysis (FMEA).

PAT (Process Analytical Technology)

According to the Food and Drug Administration (FDA), Process Analytical Technology (PAT) is "a mechanism for designing, analysing, and controlling pharmaceutical manufacturing processes by measuring critical process parameters that affect critical quality attributes of an Active Pharmaceutical Ingredient (API) during manufacturing."

In order to manage the drug development process more effectively, artificial intelligence approaches that use Machine Learning techniques have become essential. These models employ real-world information to inform their forecasts and design decisions, boosting output, uniformity, and quality in the process. The use of machine learning in the pharmaceutical industry presents a great chance to create new, more effective drug compositions. In conclusion we can say the adoption of Quality by Design principles, combined with machine learning and advanced technology, is transforming the pharmaceutical industry. With a focus on product and process understanding, risk management, and continuous improvement, QbD is paving the way for safer and more effective drug formulations in a cost-effective manner.

Pharmaceutical companies using AI

AI is rapidly transforming the pharmaceutical industry.[52-67] AI is being used to improve drug discovery, development, and manufacturing. Reverse Engineering and Forward Simulation (REFS) is a piece of machine learning software developed by GNS Healthcare that helps doctors automatically match pharmacological treatments to specific patients. It is able to forecast a patient's reaction to prospective medication treatments by analysing a variety of elements that may impact the outcomes, such as the body's capacity to absorb substances, their distribution in the body, and a person's metabolism. This ability allows it to predict how a patient will react to a medicine. For

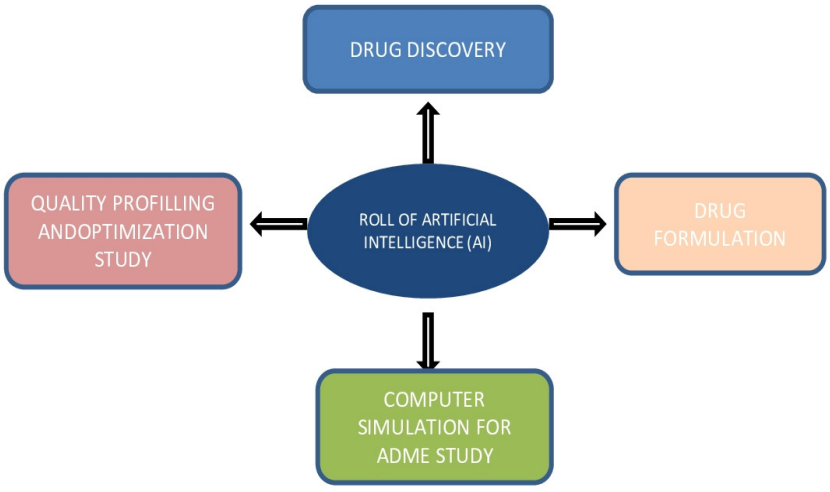

Figure 2: Application of AI in Pharmaceutical Sciences

structure-based drug design and discovery, Atom wise has created Atom Net technology, which uses deep learning neural networks. Convolutional neural networks are used, which are also found in voice and facial recognition technologies as well as in self-driving automobiles. Atom Net can learn chemical binding properties without requiring human tuning or over-parameterization since it displays molecule-protein interaction as 3D pixels with channels for distinct atoms. In the drug discovery process, Atom wise identifies regions for potential small molecules and screens them for molecules that bind to specific targets.

In silico Medicine has launched its Pharm AI project, which employs Generative Adversarial Networks (GAN) and reinforcement learning algorithms. New molecular structures may be created and the causes of illnesses can be traced with the use of these technologies. The organisation also gathers and analyses healthy and disease-affected tissue to discover patterns in the ageing process and illnesses, which helps in medication treatment development and drug scoring for efficacy assessment. New and better therapies are developed and people's access to those treatments is streamlined with the use of AI technologies at Novartis Health. Digital photographs of cells treated with various experimental substances are analysed by the company's machine learning system and then classified. In order to help researchers make better use of insights gained through their work and to forecast which untested compounds could be worth examining in further depth, machine learning algorithms can categorise compounds based on their effects. Verge Genomics uses automated data collection and analysis to combat difficult illnesses including Amyotrophic Lateral Sclerosis (ALS) and Alzheimer's. This firm uses search engine-like methods, like those developed by Google, to identify disease-causing genes and discover medications that work on numerous genes at once. Artificial intelligence software developed by Bayer and Merck & Co to aid in the management of Chronic Thromboembolic Pulmonary Hypertension (CTEPH) has been granted Breakthrough Device Designation by the Food and Drug Administration. The software analyzes image findings and a patient's clinical history to assist radiologists in identifying CTEPH patients more efficiently. IBM Watson facilitates clinicians in finding suitable clinical trials for eligible patients quickly and easily. Real-time analysis of both organised and unstructured patient medical information is performed by the software, with the result being a summary of pertinent features that may be used by physicians to narrow down the field of clinical trials for a certain diagnosis.

Apple uses AI to improve healthcare by collecting data from iPhone and Apple Watch products. This data is used to create apps for medical research through an open-source framework called Research Kit. Health Kit enables physicians to get data like heart rate and daily step count from patients' iOS devices, which might ease patient recruitment for clinical trials.

The artificial intelligence drug discovery company Exscientia partnered with Alzheimer's Research UK Oxford Drug Discovery Institute (ARUK-ODDI) in developing drugs for Alzheimer's disease.

Similarly, Genesis Therapeutics, a biotech company partnered with Genentech, a member of the Roche Group that uses artificial intelligence for drug discovery and development, has. The collaboration will use Genesis Therapeutics' graph machine learning and drug discovery expertise to identify novel drug candidates for therapeutic targets across multiple disease areas.

Bayer has entered into three-year collaboration with Exscientia Ltd., a UK-based Artificial Intelligence driven drug discovery company and to carry out research to identify and optimize novel lead structures for potential drug candidates to treat cardiovascular and oncological diseases.

CONCLUSION

AI has emerged as a powerful tool in various industries, and pharmaceutical sciences are no exception. AI is revolutionizing the way drugs are discovered, developed, and delivered, significantly impacting the pharmaceutical sector. With the increasing complexity of diseases and the need for more effective and personalized treatments, AI has become a game-changer in the pharmaceutical industry. One of the significant areas where AI is making a difference is drug discovery. Drug formulation, development requires extensive testing and optimization of various parameters. AI models can quickly analyze data from multiple experiments and identify the most promising formulations, saving time and resources. Pharmaceutical firms may reduce development times and costs for new pharmaceuticals by using AI-based optimization approaches. Absorption, distribution, metabolism, and excretion are only some of the aspects of drug behaviour that may be modelled and predicted using AI. By integrating AI models into the drug development process, researchers can gain a deeper understanding of a drug's pharmacokinetic and pharmacodynamic properties. This knowledge helps in designing drugs with improved efficacy and reduced side effects.AI also plays a vital role in drug repurposing, where existing drugs are tested for new therapeutic indications. AI algorithms can analyze large datasets of drug compounds and biological targets to identify potential drug candidates for new diseases. This approach saves time and resources compared to traditional drug discovery methods.

In conclusion we may say, AI is playing a transformative role in pharmaceutical sciences. Artificial intelligence is changing the pharmaceutical sector from the ground up, from drug research and development to customized therapy and medication production. Pharmaceutical firms may use AI's efficiency, speed, and low cost to develop and distribute new therapies to patients. As AI technology continues to advance, the future of pharmaceutical sciences looks brighter than ever.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ABBREVIATIONS

AI: Artificial Intelligence; **ML:** Machine Learning; **QSAR:** Quantitative Structure-Activity Relationship; **ANN:** Artificial Neural Network**; SVM:** Support Vector Machines; **PKPD Model:** Pharmacokinetic and Pharmacodynamic Model; **ADME:** Absorption, Distribution, Metabolism, and Excretion.

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