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ARTIFICIAL INTELLIGENCE: A NOVEL TECHNIQUE OF PHARMACY

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Abstract

Technology and computer advancements have permeated every aspect of science. One fundamental area of computer science that has influenced every field of science and technology, from basic engineering to pharmaceuticals, is artificial intelligence (AI). As a result, the fields of medicinal chemistry and health care have begun to use AI. Computer-aided drug design has supplanted traditional drug design techniques in recent years. Artificial Intelligence is being used widely to enhance drug design methods and time requirements. Additionally, AI makes it easy to identify the target proteins, increasing the likelihood that the intended medication will be successful. Artificial Intelligence has found application in de novo drug design, activity scoring, virtual screening, and in silico assessment of a drug molecule's characteristics (absorption, distribution, metabolism, excretion, and toxicity). Pharmaceutical businesses and AI companies have partnered to advance medication research and the healthcare system more quickly. It also gives a quick rundown of the pharmaceutical corporations' latest achievements in drug discovery through their partnerships with various AI firms.

KEYWORDS: Artificial intelligence, Computer-aided drug design, Drug design, Pharmaceuticals.

INTRODUCTION

The field of computer science known as artificial intelligence (AI) studies the intelligence of machines. An intelligent agent is a system that makes decisions to increase its chances of success. The study of ideas is what gives computers the ability to do actions that give the impression of intelligence. Reasoning, knowledge, planning, learning, communication, perception, and the capacity to move and manipulate objects are among the fundamental ideas of artificial intelligence. It is the engineering and science of creating intelligent devices, particularly computer programs. There are several uses for artificial intelligence in modern culture. Because it can effectively handle complicated problems in a variety of areas, including healthcare, entertainment, banking, education, etc., it is becoming increasingly important in the modern world. AI is facilitating faster and more comfortable daily living. Artificial intelligence seems like the best option for us with its many applications and advantages. While the new paradigm of non-biological computing and intelligence is expanding exponentially, biological intelligence remains fixed since it is an old, established paradigm. Approximately ten thousand million binary digits could be stored in the human brain. However, most of the information is presumably utilized in other somewhat wasteful ways, such as recalling visual impressions. Because natural intellect is finite and unpredictable, we can conclude that the modern world may rely heavily on computers. Artificial intelligence (AI) is expected to become a fundamental feature of all contemporary software in the upcoming years and decades, making it a genuinely revolutionary advancement in computer science. This poses a risk, but it also offers a chance. Artificial Intelligence will be used to support both offensive and defensive cyber operations. Furthermore, new methods of cyberattack will be developed to exploit the unique flaws in AI technology. Lastly, AI's voracious appetite for massive volumes of training data will increase the value of data and redefine our needs when it comes to data protection. Globally prudent governance will be necessary to guarantee that this revolutionary technology will result in prosperity and safety for all. (1)

Artificial intelligence is still a relatively new field. In the 1950s, scientists and researchers started to speculate about the prospect of computers processing human-like intellectual capacities, which led to the development of artificial intelligence as a field of study. The British mathematician Alan Turing was the first to suggest a test for identifying an intelligent machine. Later on, the test was dubbed the Turing Test, in which a machine attempts to pass for a person in an imitation game by responding to questions in a way that is similar to that of a human. Turing thought that a machine could be regarded as intelligent as a human being if it could fool a human into thinking that it was speaking with another person. In 1956, John McCarthy, a professor at the Massachusetts Institute of Technology, coined the term "artificial intelligence."

The phrase was coined by McCarthy for a conference he was hosting that year. AI researchers later dubbed the conference the Dartmouth Conference, and it helped to establish AI as a separate field of study. The conference also outlined the main objectives of AI, which are to create machines that think like people and to comprehend and simulate human thought processes. Between 1956 and 1966, a large portion of AI research was theoretical in character. Mathematical theorems could be proved by the first artificial intelligence software, the Logic Theorist (displayed at the Dartmouth Conference). Later, a number of other systems were created by utilizing AI, like "Sad Sam," which was created by Robert K. Lindsay in 1960 and could comprehend basic English sentences as well as make inferences based on information exchanged during a conversation. The data, which in AI is referred to as the knowledge base (KB), influences the conclusions reached. Another was ELIZA, a program Joseph Weizenbaum created at MIT in 1967 that could mimic a therapist's reactions to a patient. As the viability of AI was further demonstrated, the focus of AI research changed. The definition of artificial intelligence that is used today—"a variety of research areas concerned with extending the ability of the computer to do tasks that resemble those performed by human beings"—was born out of this shift in research focus, according to V. Daniel Hunt's 1988 article "The Development of Artificial Intelligence" (Andriole 52). Expert systems, neural networks, and robotics are a few of the most fascinating topics in AI study today. (2)

FEATURES OF IDENTIFYING OPTIMIZATION PROBLEMS OF MODERN INDUSTRIAL PRODUCTION

Systems thinking is based on the scientific concept of cybernetics. All of the system's indivisible components are connected to one another. Many different types of masked agents are permitted in the theories of automated control, discrete mathematics, and digital automata. These agents are defined, but they lack a relational core. Furthermore, one of the features of the difficulty of recognizing production problems is the dichotomous nature of the definition. Manufacturing can be thought of as a system operating in a dynamic environment, on the one hand. However, cybernetic control itself can be thought of as a system. Furthermore, if the process value is fixed at this point, then the development of the process after any given value is independent of evolution, the "predecessor" (the "future" of the process depends on the "past" only through the "present"). The evaluation of the posterior maximum in Markov systems including cybernetic systems is contingent upon the knowledge of individuals who possess preconceived notions about the environment and circumstances of employment. This is the issue of figuring out modernization and production optimization issues. This is a result of the law enforcement profession, which is represented in an already-classic design approach to the creation and upkeep of automated control systems. This is decided by the factoring side's priority examination of the enterprise's dynamics. The more straightforward econometric side and economic transparency mandate this. Because an enterprise's challenges are mostly financial in nature, economists and financiers are required to provide solutions. Specialists with this training profile, however, are not able to look at the business as a whole. As a result, emphasis is drawn to a significant omission and the failure to apply a single, straightforward analytical technique to the issues raised. After all, the "optimization" of a system is only appropriate when it simplifies the system to its most basic form without affecting its functionality in any manner. Put differently, every management strategy that is put into practice is linked to an optimality standard. There are two types of optimization methods: iterative and direct. The goal of optimization is to identify the best choice. They are used to determine the ideal time for technological processes, the best geometric design, the optimal technology, and related duties. Newton's iterative approach is one illustration of this. The enterprise's information security and economics principles must be the foundation for identifying issues that prevent particular optimization. The process of updating and upgrading production is not directly linked to security, but it can address the issue of selecting the best tools, techniques, and means of cognitive effect on control devices and subordinate aggregates. As a result, we will identify two categories of potential risks to the industrial sector's ability to update, modernize, and optimize its technical processes:

- Entropy of the "control device" is the naive idealization of general predictability and presumed linearity in operation. Though not restricted in its use, linearization is feasible.
- An economic approach to innovation strategy that just considers the financial aspects of projected losses and gains, depreciation (3)

EVOLUTION OF SUB-DISCIPLINES OF ARTIFICIAL INTELLIGENCE

1. ARTIFICIAL INTELLIGENCE AND COMMUNICATION

With the high level of ICT use in the communications industry and the range of customer demands it faces regarding personalization, multimedia services, and precision management, network security is becoming increasingly crucial. The benefits of artificial intelligence (AI) in learning, comprehending, reasoning, and collaborating have been gradually revealed. As a result, deep packet inspection and service-aware network technologies are nearly mature, and the intellectualization of communication networks and services is becoming feasible. Software-defined networks (SDN) and network functions virtualization (NFV) have also emerged. Additionally, operators are very interested in AI since it could reduce operating and capital investment costs (OPEX and CAPEX). Different interests, routines, and information needs of businesses and individual users are gradually exposed as the number of users and the communication network expand. Since enterprise users may now access customized networks and services, there is an increasing need for specialist firms. Every user will receive a unique service package and possibly a unique network in the future. It would be impossible to meet such complicated standards without an intellectual tool. With the advent of the Web 2.0 era, users of the Internet are becoming both producers and consumers of information, and they are creating an increasing amount of multimedia content. Internet traffic is increasing at an incredible rate because of user-generated content. Both transmission and storage are extremely difficult in these conditions. AI's incorporation strengthens our capacity to meet this challenge. The diverse dimensions and granularities in today's wireless traffic models must be taken into account in the networks due to the widespread usage of smartphones. Network management has gotten more accurate with the emergence of software-defined networks and network function virtualization technologies. Virtualization applies not just to network parts but also to individual components like CPU, memory, ports, bandwidth, etc. With the help of AI-based technology, operators can create on-demand networks just for certain consumers. Using AI, operators can achieve other objectives in addition to reducing their energy consumption. In order to handle intricate resources and constantly changing traffic, operators must make wise choices. However, there is currently no one model that can adequately capture the features of network traffic. AI is also capable of automatically picking up features like data flow, management, controls, and other features, as well as developing expert knowledge of running, managing, and maintaining networks. The structure of communication networks is becoming more and more complex as a result of the network's growth in both size and scope. In network administration, terms like hierarchy and distribution are frequently used. All network nodes are assigned management tasks and controls. This means that we have to deal with problems like task distribution and coordination between management nodes. We can anticipate the capacity for cooperation between network managers dispersed throughout all tiers if we incorporate distributed artificial intelligence's multi-agent collaboration feature into network management.

The sensor and FINE executor is the DPI probe. It first determines the state of the thing it is accompanied by. It gathers any pertinent data from the object it is accompanied by and transmits it, via the agent, to the AI plane. Second, it carries out directives from the intelligence plane and takes autonomously determined essential actions. Infrastructures and systems for user services, communication networks, management systems, etc. are examples of service components. The manager may be assisted by management systems such as OSS, BSS, NMS, EMS, etc. SDNs/NFVs, conventional networks, etc. are examples of communication networks. Cloud computing, mobile Internet, data communications, 5G, and other systems are examples of user service systems. Infrastructures comprise hardware, data centers, etc. (4)

2. ARTIFICIAL INTELLIGENCE IN HEALTH CARE

Systems with artificial intelligence have demonstrated the ability to enhance physicians' interpretation and ensuing decision-making. However, the growing accountability gaps and the increased danger of unfavorable side effects that come with medical treatments outweigh the potential advantages of this capability. Essentially, current clinical accountability models and safety assurance procedures are under pressure as digital health systems expand their reach and power. The issues pertaining to safety assurance and moral accountability might be attributed to the unwillingness of safety-critical industries, such as nuclear power and aviation, to consider applying artificial intelligence in their operations.

The Artificial Intelligence (AI) Clinic, a proof-of-concept system that employs reinforcement learning to suggest actions for the care of patients fulfilling the third international consensus definitions for sepsis and septic shock, was created by Imperial College London researchers in an effort to help address the problem of optimizing treatment. Since the 90-day mortality rate for these individuals is about 20%, the software of the system is taught to prevent deaths. The system simulates clinical decision-making by analyzing 48 features from an electronic patient record and applying a Markov decision process. It then recommends fluid and vasopressor doses in broad ranges for each 4-hour window. Although the system is now being tested off-policy (without heeding its advice) and was designed using retrospective data, its researchers want to conduct prospective studies in the future. We highlight the main gaps in safety assurance and moral accountability brought about by this kind of AI-based capabilities in the following two parts. The clinician doesn't only pick a goal for blood pressure; rather, it operates without any set target at all and provides recommendations for individualized treatment based empirically on the results of thousands of individuals. Research has demonstrated that human clinicians are susceptible to clinical inertia, which is the tendency to stick with a treatment plan even in the face of changes in the patient's clinical picture, and can be sidetracked by conflicting demands at work. In contrast, the digital system continuously monitors and offers personalized recommendations every four hours. It's crucial to remember, though, that it's unclear if a doctor's inertia always has a negative impact on patient care.

A mathematical model of outcomes that are partially random and partially governed by choices the system makes along the way is called a Markov decision process. As a result, while making decisions, AI Clinicians disregard the system's past states and may even defy standard clinical practice by abruptly altering vasopressor dosages. Since AI Clinician is an assistive technology, the system is not responsible for handling every clinical task. The human clinician overseeing the patient's treatment makes the final choice. However, the interpretation of data—a crucial, cognitive component of the decision-making task—is outsourced. When even a small portion of the decision-making process is delegated to a machine, the control and epistemic conditions of accountability are compromised. The following further jeopardizes the control state. The sepsis itself, the existence of variables including novel medications, novel diagnoses, novel germs, and novel viruses, as well as variations in patient care at prior periods, all influence how complicated the clinical environment is. Nonetheless, it is challenging to simulate the clinical situation in the computational model when the technology is still in the design stage. Because it was not possible to adequately express the clinical intentions on the system, the software's behavior might not accurately reflect such aims. In order to address this issue, certain components of the procedure are being ignored (for instance, by reducing the amount of information inputs compared to those obtained by human doctors). However, unforeseen repercussions might occur. For instance, insensible fluid losses are not recordable electronically, which may cause the machine to recommend additional fluids even when a clinician can see that the patient is already dehydrated. Moreover, it is possible for the machine to interpret the data in a manner that deviates from the human clinician's understanding of what matters most in the particular situation. For instance, a physician may decide to disregard a very unusual blood test result that might have been the consequence of a mistake in the test's processing, transcription, or blood sampling.

For a variety of reasons, it is challenging to comprehend the epistemic state of best practices when it comes to treating sepsis in hospitals. First, there are numerous methods that medical professionals employ to treat sepsis. Second, there could be variations in the approaches taken by nurses and doctors. While nurses are in charge of minute-by-minute adjustments to treatment, clinicians establish the overall framework of the plan. Thirdly, there is the fact that best practices are subject to change due to new diseases and treatments that raise concerns about what constitutes optimal care as well as changes in our understanding of what constitutes ideal therapy (such as the shift from administering fluids to using vasopressor medicines). Two aspects of the computer itself further jeopardize the epistemic condition: first, its own incomplete interpretation of the operating environment; second, many of its decisions are opaque, even to the designers and users. The implicit commitment that physicians and healthcare organizations make to patients—to use sound judgment, behave competently, and deliver healing—is a fundamental component of any complicated healthcare system. Moral responsibility supports the patient's faith in the treating clinician and keeps professionals from becoming complacent in their work. Patients typically think that the therapist is behaving in a kind manner toward them. But benevolence has no bearing on the choices made by a computer program. It would make sense for a patient to desire to know why an artificial intelligence system's advice was adopted if human clinicians are not in complete control of the system or are unaware of its recommendations.

Since human clinicians still make the final choice, we can characterize the artificial intelligence system as merely advisory and assume that accountability is thereby secure. But doing so can lead to a predicament where there are two equally bad options. The artificial intelligence system offers little value if therapists have to take the time to form their own ideas on the optimal course of action. Alternatively, if clinicians accept the advice without question, the control and epistemic requirements of moral accountability are further undermined. A similar conundrum impacts safety assurance in that the system being confirmed now includes the physician, making it impossible to assure the system in isolation. Safety assurance becomes more and more crucial to both clinicians and patients when there is no direct and purposeful control over the suggestions made by an artificial intelligence system and because many of these systems are opaque. Safety assurance gives users reason to believe that the system's associated patient safety risk is kept as low as is practical. Nevertheless, the majority of current safety examples are static, which is incompatible with the dynamic nature of clinical settings and machine learning. Artificial intelligence systems' adaptive behavior usually modifies the clinical setting, refuting the safety case's presumptions. It follows that the concrete specification which is used to create the system and which the system implements cannot fully describe the intended function. The specification is predicated on a small number of data points (vital signs and laboratory results), in this case, the treatment of sepsis in intensive care. Because of this, it is far more difficult to guarantee that the system's intended function maintains safety in every clinical circumstance in which it will operate using a static safety case. The actual risk of injury to patients is becoming harder to determine, and this problem poses an epistemological challenge to safety engineers. The safety engineer faces a control issue while trying to minimize the real risk of injury to patients. From a technical engineering standpoint, robustness—the characteristics of the system that could impair its availability and performance but would not directly cause patient harm—is frequently the only factor taken into account when discussing the safety of artificial intelligence. Overfitting of the predictive model is one instance, in which the model is unable to generalize outside of the original data set. The relationship between these technological characteristics and patient harm is frequently overlooked by technologists. One such example is the possibility that biases in artificial intelligence training data could jeopardize the accuracy of diagnoses in specific minority communities. (5)

3. Artificial Intelligence (AI) in Pharmacy

Artificial Intelligence (AI) has become a popular remedy for issues involving numbers and data. Numerous technological advances have resulted from this discovery in almost every industry, including engineering, architecture, education, business, accounting, health, and so forth. It has made great strides in the healthcare industry. It has been instrumental in the management and storage of data and information, including patient medical histories, medication inventories, sales records, and more; in automated machinery; and in the development of software and computer applications, including diagnostic tools like CT diagnosis and MRI radiation technology. Without a doubt, artificial intelligence (AI) has transformed healthcare to be more effective and efficient, and the pharmaceutical industry is not exempt.

AI is used in hospital-based healthcare systems in a variety of ways, including determining appropriate or available administration routes or treatment strategies, organizing dosage forms for individual patients, and more.

- **Health support and medication assistance**

Artificial intelligence (AI) has gained recognition as an effective tool for pharmaceutical assistance and health support services in recent years. A kind face and a nice voice greet Molly, a virtual nurse created for a start-up. Its goal is to support patients with their chronic ailments during doctor appointments and assist them in directing their own treatment. A software called AI Cure that works with a smartphone's webcam tracks patients and helps them take charge of their health. Patients who take part in clinical trials and those with severe drug conditions can both benefit from this app.

- **Accuracy of medicine**

AI has a positive effect on genetic development and genomics. Using patterns found in genetic data and medical records, Deep Genomics, an AI system, can be used to find mutations and their connections to diseases. This technique provides physicians with information on what happens inside a cell when genetic variation modifies DNA. Craig Venter, the creator of the human genome project, created an algorithm that uses a patient's DNA to provide physical traits. When cancer and vascular disorders are still in their early stages, "Human Longevity" AI technology can be used to pinpoint their precise location.

- **Maintaining medical records**

It is a difficult undertaking to maintain patients' medical records. Putting the AI system into practice makes data collection, storage, normalization, and tracing simple. Short turnaround times for the extraction of medical records are facilitated by Google's Deep Mind health project. For quicker and better medical care, this project is therefore helpful. This project is supporting the Moorfields Eye Hospital NHS in its efforts to enhance eye care.

- **Assisting in repetitive tasks**

AI technology also helps with some repetitious activities, such as analyzing radiography, ECHO, ECG, and X-ray imaging to identify and detect diseases or abnormalities. An algorithm developed by IBM called Medical Sieve is a "cognitive assistant" with strong analytical and reasoning skills. In order to combine deep learning with medical data and enhance the patient's condition, a medical startup is required. For every bodily component, there is a separate computer program that is employed in a certain illness state. For practically any kind of imaging analysis, including X-ray, CT, ECHO, ECG, etc., deep learning can be used.

- **Treatment plan designing**

AI technology makes it feasible to create treatment programs that are both effective and efficient. An artificial intelligence (AI) system is required to take control of the situation when a patient develops a severe condition and choosing an appropriate treatment plan becomes challenging. This technology takes into account all of the prior data and reports, professional experience, etc. when creating the recommended treatment plan. With the help of insights gained from working thousands of hours with physicians at Memorial Sloan Kettering Cancer Center, IBM Watson for Oncology is a cognitive computing decision support system that analyzes patient data against thousands of historical cases and offers treatment options to assist oncology clinicians in making educated decisions. (6)

4. **Artificial Intelligence in Drug Discovery and Development**

Since the preclinical, pharmacokinetic, pharmacodynamic, and toxicological studies encompass a multitude of in silico, in vitro, and in vivo experimentations that typically span several years, the development of a new drug is an extremely drawn-out and expensive procedure. In this study, we provide a brief overview of several published cases that highlight the effectiveness of computer-assisted drug development processes and highlight the useful applications of artificial intelligence (AI) technology in this exciting field. In addition, we discuss the issue of medication repurposing in clinical settings. However, there aren't many examples of this kind of achievement, which shows us that AI has a lot of potential for speeding up the discovery of new, effective drugs. AI methods are completely essential and vital instruments in the creation of novel medicines, and AI speeds up the process of repurposing existing drugs. Even though the use of AI in drug research is still in its infancy, the potential for breakthroughs in AI and machine learning (ML) algorithms is enormous. Pharmaceutical scientists, computer scientists, statisticians, physicians, and other professionals are driving AI/ML solutions that are accelerating collaboration in drug development processes and the adoption of AI-based technology for the quick identification of new medications. Big data and AI techniques are anticipated to significantly increase the efficacy of medication repurposing and the discovery of novel medications for a range of complicated human illnesses.

- **Artificial intelligence yields new antibiotics**

Researchers at the Massachusetts Institute of Technology (MIT) identified a medication called halicin that kills a variety of bacterial strains using a machine-learning algorithm. In E. coli, halicin inhibited the growth of antibiotic resistance. Many of the most dangerous infectious disease-causing bacteria in the world, including some types resistant to all known antibiotics, were eliminated by the medication in laboratory tests. Additionally, it eliminated infections in two distinct mouse models. The study published in Cell discovered that E. coli did not become resistant to halicin during the course of a 30-day treatment period. In an effort to develop halicin for use in people, the researchers intend to continue additional studies on the drug in collaboration with a nonprofit or pharmaceutical firm.

- **Development of potent anti-plasmodial using artificial intelligence**

Artificial intelligence (AI) using a variety of models has proven to be very accurate in the field of chemical property prediction. The AI model would identify trends in the data and aid in the effective search for hit chemicals. The authors of this paper introduced DeepMalaria, a deep learning-based procedure that uses a compound's SMILES (Simplified Molecular-Input Line-Entry System) to predict its anti-Plasmodium falciparum inhibitory characteristics. 13,446 publicly accessible antiplasmodial hit compounds from the GlaxoSmithKline (GSK) dataset are being used to train a graph-based algorithm, which is then utilized to identify new malaria treatment candidates. According to experiments, one of the compounds' mechanisms of action, DC-9237, not only inhibits all asexual phases of Plasmodium falciparum, but it also acts quickly, making it a promising option for additional study. (7)

5. **Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design**

Artificial intelligence (AI) has become a potent instrument that utilizes personal knowledge and offers quicker fixes for difficult problems. Significant developments in artificial intelligence (AI) and machine learning offer a game-changing chance for drug discovery, formulation, and dosage form testing. Through the use of AI algorithms, researchers may find targets linked with disease and anticipate how those targets would interact with possible drug candidates by analyzing large amounts of biological data, such as proteomics and genomes. This makes it possible to approach drug discovery in a more effective and focused manner, which raises the possibility of successful drug approvals. Additionally, by streamlining the research and development process, AI can help lower development costs. In addition to helping with experimental design, machine learning algorithms can forecast the toxicity and pharmacokinetics of potential drugs. This capacity lessens the need for expensive and time-consuming animal testing by allowing the prioritization and optimization of lead compounds. Artificial intelligence (AI) algorithms that examine actual patient data can support personalized medicine strategies, improving patient adherence and treatment outcomes. The broad range of uses of AI in drug discovery, drug delivery dosage form designs, process optimization, testing, and pharmacokinetics/pharmacodynamics (PK/PD) research are examined in this thorough overview. This analysis highlights the advantages and disadvantages of the several AI-based strategies used in pharmaceutical technology. However, the pharmaceutical industry's ongoing exploration and investment in AI present great opportunities for improving patient care and drug development procedures. (8)

List Of Commonly Used AI Models in The Pharmaceutical Industry. (8)

AI/Machine	**Learning Models Description/Usage**
Generative Adversarial Networks (GANs)	In order to produce unique chemical compounds and maximize their attributes, GANs are commonly used in the creation of medicinal products. GANs produce structurally varied and functionally optimal drug candidates by combining a discriminator network to assess the quality of newly created molecules with a generator network to generate new ones.
Convolutional Neural Networks (CNNs)	CNNs work well for image-based tasks such as drug target identification and molecular structure analysis. They can help with target identification and medication design by extracting pertinent information from molecular pictures.
Recurrent Neural Networks (RNNs)	In drug development, RNNs are frequently used for sequence-based tasks such as peptide sequence design, genomic data analysis, and protein structure prediction. They are able to create new sequences based on patterns they have learned and record sequential interdependence.
Long Short-Term Memory Networks (LSTMs)	LSTMs are a type of RNN that excels in modeling and predicting temporal dependencies. They have been used in pharmacokinetics and pharmacodynamics studies to predict drug concentration-time profiles and evaluate drug efficacy.
Transformer Models	In the pharmaceutical industry, transformer models—like the well-known BERT (Bidirectional Encoder Representations from Transformers)—have been used for natural language processing tasks. Researchers can make educated decisions on the development of new drugs thanks to their ability to extract valuable information from clinical trial data, patent databases, and scholarly literature.
Bayesian Models	In the process of developing new drugs, Bayesian models like Gaussian processes and Bayesian

	networks are used to quantify uncertainty and make decisions. They let scientists evaluate risks, create more effective experimental designs, and make probabilistic predictions.
Deep Q-Networks (DQNs)	Deep QNs (a hybrid of deep learning and reinforcement learning) have been applied to predict compound activity and identify high-potential candidates for additional testing, thus optimizing drug discovery procedures.

Popular AI model tools used for drug discovery. (8)

AI Model Tools	Summary
Deep Chem	An open-source library offering a large selection of drug discovery tools and models, such as generative chemistry, virtual screening, and deep learning models for molecular property prediction
RDKit	A popular open-source cheminformatics library with several features for managing molecules, finding substructures, and calculating descriptors. It is compatible with machine learning frameworks for applications related to drug development.
ChemBERTa	A linguistic paradigm was created especially for tasks involving drug development. Based on the Transformer architecture, it can synthesize molecular structures, forecast attributes, and help optimize leads thanks to pre-trained training on a substantial corpus of chemical and medicinal literature.
GraphConv	An architecture for a deep learning model that uses molecular graphs. It has proved successful in foretelling chemical attributes by using the structural data contained in the graph representation of molecules, such as bioactivity and toxicity.
AutoDock Vina	A well-known docking program that forecasts the binding affinity of small compounds and protein targets using machine learning approaches. It can help with lead optimization and virtual screening in the context of drug discovery.
Schrödinger Suite	A full-featured drug discovery software suite that includes a number of AI-powered capabilities. It has modules for virtual screening, ligand- and structure-based drug design, predictive modeling, and molecular modeling.
IBM RXN for Chemistry	Chemical reaction prediction using an artificial intelligence model. It helps in the identification of new synthetic pathways and compound synthesis by generating possible reaction outcomes using deep learning algorithms and massive reaction databases.

Scape-DB	A database called scape-DB (Extraction of Chemical and Physical Properties from the Literature-DrugBank) uses machine learning and natural language processing to extract biological and chemical information from scholarly publications. It offers useful data for the study of drug discovery.

LIST OF COMMONLY EXPLORED AI MODELS IN PHARMACEUTICAL PRODUCT DEVELOPMENT (8)

AI/Machine	**Learning Models Description/Usage**
Genetic Algorithms	Genetic algorithms are optimization methods derived from the ideas of genetics and natural selection. To obtain the required dosage form properties, they can be used to improve drug release patterns, formulation compositions, and process parameters.
Artificial Neural Networks (ANNs)	ANNs have been used to simulate and improve the kinetics of medication release at various dose forms. They can help determine the best possible formulations and forecast how active pharmaceutical ingredients (APIs) will be released under different circumstances.
Monte Carlo Simulation	Through the consideration of uncertainties and variability in formulation and process factors, drug product performance has been optimized through the use of Monte Carlo simulation methodologies. They support the creation of robust formulations and processes.
Computational Fluid Dynamics (CFD)	The optimization of fluid flow and mixing during dosage form production procedures, such as granulation, coating, and drying, is made possible using CFD simulations. They support the creation of consistent, effective processes.
Response Surface Methodology (RSM)	RSM is a statistical method that models and examines the link between several variables and how it affects formulation responses to help optimize dosage form formulations. It facilitates comprehending and refining formulation parameters.

Algorithms are used for the development of AI models for various PKPD studies (8)

Algorithm/Software	Aim/Target	Advantage	PK/PD /Both
Bayesian/WinBUGS	To manage information below the quantifiable limit	• Simple implementation • Previous knowledge from the literature can be used directly for model-fitting	Both
Support Vector Machine/Least Square-SVM	Drug concentration analysis using a sample drug according to each patient's unique profile	• Customized model for each new patient • SVM-based techniques outperform PK modeling in terms of drug concentration prediction accuracy.	PK
Drug Target Interaction Convolutional Neural Network (DTICNN)	Determining the interactions between drugs and targets and forecasting possible drug compounds	• Economical • Time-saving	PD
Linear Regressions (LASSO)/Gradient Boosting Machines/ XGBoost/Random Forest	Time series and area under the concentration are used to predict the plasma concentration versus time curve from 0 to 24 hours following consecutive doses of Rifampicin	Analysis that saves time and enhances the covariate selection process	PK
XGBoost	Calculating the drug's area under the curve (AUC) for mycophenolate mofetil (MMF) or tacrolimus	Pharmacokinetic (PK) datasets from patients undergoing liver, heart, and kidney transplants were reliably predicted.	PK

6. Artificial Intelligence (AI) Technologies Used in the Development of Solid Dosage Forms

One strategy that shows promise for speeding up the development of new medicinal products is formulation development based on artificial intelligence (AI). AI is a flexible tool with a variety of algorithms that can be used in different situations. Tablets, capsules, powder, granules, and other solid dosage forms are some of the most commonly utilized types of administration. Critical material attributes (CMAs) and processing parameters are two of the many variables that can impact product properties during the product development process. These features include dissolving rates, particle size distribution, physical and chemical stabilities, and the dry powder's aerosol performance. But the traditional trial-and-error method of product creation is ineffective, time-consuming, and arduous.

Artificial Intelligence has garnered significant attention as a novel and innovative method for developing pharmacological formulations. The following analysis offers the following insights: a general overview of artificial intelligence (AI) in the pharmaceutical sciences and the main regulatory agency guidelines; methods for creating a database of solid dosage formulations; knowledge of data processing and preparation; a synopsis of and comparison of AI algorithms; and details on applications and case studies of AI in relation to solid dosage forms. Furthermore, the potent method known as deep learning-based image analytics will be covered, along with its potential uses in the pharmaceutical industry. (9)

One of the most often used deep learning algorithms in the pharmaceutical business is the ANN. The input, hidden, and output layers make up an ANN. There are a certain number of neurons in every layer. In an artificial neural network (ANN), neurons are utilized to transmit signals and biologically mimic the human brain. Another well-liked deep learning algorithm that is more frequently employed for image processing is a convolutional neural network (CNN). Convolutional, pooling, flattening, and buried layers are components of a traditional CNN. CNNs have been extensively utilized for problems related to image classification and segmentation, thanks to advancements in computational technology like GPU and CPU.

In the 1990s, scientists and researchers started looking into the use of AI in solid dosage forms. The body of published research indicates that since 2015, the number of publications on AI in solid dosage forms has grown by 100% yearly. Tablets are the most popular solid dosage form among all of them, accounting for more than 60% of all AI-related solid dosage form development. Convolutional and recurrent neural networks are two examples of DL algorithms that have been successfully applied in the pharmaceutical sciences recently for a variety of uses when creating solid dosage formulations, including detecting tablet defects [64, 65], forecasting storage stability, forecasting particle flowability, and forecasting drug dissolution profiles. Algorithms created in programming languages like Python, Lisp, C^{++}, JavaScript, Java, and Haskell are used to carry out the AI modeling process. Furthermore, various machine learning tasks can be implemented using a variety of commercially available tools and platforms, such as IBM Watson, TensorFlow, Cortana, Azure Machine Learning Studio, and Google Cloud Machine Learning Engine. Scientists can now anticipate key elements of medication compositions with the aid of AI technology, which enhances the process of developing new products by cutting costs and time. The remaining portion of this section will discuss three published research that employed AI to forecast the drug release profiles, disintegration times, and dissolving profiles of different kinds of tablets. (9)

Applications of AI in Solid Dosages Forms

Dosage Forms	Applications	Algorithms
Tablet	• Estimating the release of drugs • The creation of 3D-printed tablets • Finding tablet faults • Calculating the rate of disintegration • Medication particle size examination	• ANN, SVM, Ensemble of Regression Trees, and decision tree • ANN, self-organizing maps, RF, SVM, and CNN • CNN, You Only Look Once v5 (YOLOv5) • RF, XGBoost, ANN, • Pattern recognition neural network
Capsules	• Recognizing capsule faults • Identifying the pellet faults inside the capsules	• KNN, SVM, and CNN • SVM
Solid dispersions	• Estimating the chemical or physical stability of substances • Forecasting dissolution profiles and rates	• ANN, SVM, RF, LightGBM, KNN, and naïve Bayes • RF, SVM, LightGBM, and XGBoost
Granules	• Control of the granulation process • Forecasting the distribution of particle sizes	• Genetic programming and neuro-fuzzy logic • Genetic programming, multivariate linear regression, and ANN

7. **Artificial intelligence in pharmacology research**

Artificial intelligence (AI) is the use of data and algorithms to carry out tasks that would typically need human intelligence. Artificial Intelligence (AI) and its fundamental component, machine learning, contextualize data and improve decision-making to revolutionize medication discovery and development. It takes an ecosystem of digital data gathering, standardized procedures, complementary technology, and an ethical framework to transform clinical pharmacology (CP) into AI-augmented CP (AI/CP). Therapeutic drug monitoring provides dose recommendations for medications with a narrow therapeutic index and rather considerable PK variability in clinical practice. When predicting the bispectral index during anesthesia, AI/ML has outperformed traditional modeling methods in providing better dose recommendations for propofol and remifentanil with less error.Six AI/ML techniques are currently able to uncover patterns through the identification of intricate and nonlinear interactions as well as the impact of extrinsic and intrinsic factors on the variability of PK in various subpopulations. We believe that combining ML power with population-based methods will contribute to our understanding of PK variability and provide choices for dose adjustments in patient subgroups.

AI implementation in CP is based on the rapidly increasing digitization of the industry. AI has the potential to enhance dose recommendations—which are the primary CP deliverable—and boost pharmacometrics' effectiveness in light of the data and digital systems' change. Overall, by including expected DDI and unknown adverse effects in the CP portion of the label, the patient stands to gain. However, in order for AI in CP to be successful and flourish, concerns with ethical data sharing and a lack of causal inference must be resolved. (10)

Summary of examples featuring artificial intelligence and clinical pharmacology (10)

Description	Clinical pharmacology feature
PK/PD modeling Latent hybridization model integrating expert PK/PD models with hospital observation data through neural ODEs	PK/PD model improvement based on clinical observation factors; expert pharmacological models to support clinical decisions
Apply machine-learning algorithms to develop population PK models	Great potential for choosing PK models automatically
An automated tool to distill closed-form ODEs from observed trajectories	Finding a set of interpretable differential equations that matches a drug's PK/PD model
Non-pharmacometric models to predict longitudinal changes in tumor size	Predict changes in tumor trajectory and optimize the treatment options
Safe efficacy exploration dose allocation: a model for maximizing the cumulative efficacies while satisfying the toxicity constraints with high probability	Modern clinical designs that maintain the study's validity while determining the ideal dose at phase I with a greater success rate and fewer patients
A Bayesian framework for finding the maximum tolerated dose for drug combinations in the presence of safety constraints	Improved clinical designs that evaluate the majority of optimal dose combinations with a limited number of patients in a method that is efficient, safe, and informative
Algorithm exploring different dosing regimens for cancer treatment	Potential for personalized dosing regimen balancing safety and efficacy
A state space model for disease progression that can build on the entire patient history as opposed to the current state only	Depending on the disease's stage, improved drug delivery regimens could be found using the progression of the illness.
A machine-learning method for partitioning patients into subgroups with uncertainty quantification	Depending on the disease's stage, improved drug delivery regimens could be found using the progression of the illness.

8. **Artificial Intelligence in Chemistry**

Chemistry and artificial intelligence have a close relationship. Artificial intelligence can be used in the fields of chemistry to create novel molecules, identify molecules and compounds' chemical properties, find drugs, synthesize and retrosynthesis molecules, and forecast analytical results for more precise and better outcomes. By eliminating the least useful and unwanted findings, artificial intelligence can assist in the separation and combination of molecules using pre-existing databases, producing unique and different results.

Artificial intelligence finds uses not only in chemical labs but also in the pharmaceutical, medical, and biochemistry industries, as well as in improved analytical techniques and other related fields. It can detect, compare, and predict the molecular properties of new compounds using pre-existing databases, which speeds up research and comparison and yields effective findings. The four domains that were specifically stressed in Chemical Product Engineering (CPE) were designing and discovering new molecules or materials, predicting and choosing reaction pathways for molecule synthesis and retrosynthesis, modeling processes, and providing support for sensorial analysis. Artificial intelligence reduces the time and energy required for the massively efficient and accurate retrosynthesis of molecules in a shorter amount of time. AI algorithms aid in the prediction of likely and accurate analytical techniques, resulting in quick and precise results. In order to categorize active and inactive substances according to their capacity to inhibit SAM-dependent methyltransferases, a deep learning-based neural network model was created. The preparation of resins with a certain strength and viscosity takes longer since there may be additional factors involved, such as diols and diacids connected to the polyester group or the dilution solvents utilized. The polymer's conformational structures alter in tandem with its characteristics. With the use of AI, these can all be completed using the QSPR approach.

Moreover, AI is crucial to spectrochemistry. These days, there are many databases accessible that make it easier to quickly evaluate and analyze new compounds. In addition to studying the atomization energies of organic compounds based on their nuclear charges and atomic locations, quantum chemistry in conjunction with artificial intelligence or machine learning is helping to explore the spaces surrounding and within chemical molecules. A hexapod was used to attach the Planetary Instrument for X-ray Lithochemistry (PIXL) to Perseverance's robotic arm. AI is used to steer the PIXL to acquire the most precise aim for its X-ray beam, which is used to identify the textures and structures of rocks. Additionally, NASA fitted the rover with a SuperCam, which allowed AI to recognize, zap, and evaporate rock targets using a pulsed laser in order to examine their chemical composition. Chemical space and chemical reaction mapping can be accomplished by attention-based neural networks. (11)

CONCLUSION

Artificial intelligence (AI) is changing almost every facet of society, including the health care sector and all of its subsidiary industries. It has the potential to transform medication administration, enhance patient outcomes, and expedite pharmacy operations, even though many state laws and regulations pertaining to pharmacy practice have not yet taken into account AI and its implications. AI's introduction opens up a whole new world of possibilities and hazards. It is imperative that regulators and stakeholders comprehend the ramifications of utilizing this novel phenomenon. But it's crucial to make sure AI is applied morally and sensibly, and that its effects on society and the workforce are properly evaluated. The primary advantage of incorporating artificial intelligence (AI) into certain pharmacy applications is increased precision and effectiveness in patient treatment. In summary, this article will shed light on the pharmacy industry's future and the revolutionary potential of artificial intelligence in this domain.

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