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Review Article

Digitech World of Pharmacy through the applications of Artificial Intelligence: A Scoping Review

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ABSTRACT

Artificial intelligence (AI) is an emerging discipline in computer sciences where a computer or robot controlled by a computer performs the tasks that are associated with human intelligence. AI systems are useful in automated decision-making through Deep Learning (DL), Natural Language Processing (NLP), and Machine Learning (ML) techniques. AI has a wider range of applications in advanced web search engines, gaming, self-driving cars, recommendations, etc. As AI has spread its wings to the pharmacy field, it may be used in research and development, drug discovery, drug screening, target identification and validation, prediction of synergism and antagonism, clinical trial design, clinical diagnosis, and personalized medicine inpatient care. DeepChem, DeepNeuralNetQSAR, DeepTox, Neural Graph Fingerprint, ORGANIC, and Potential Net are used in the drug discovery process. Image-aided surgeries, Computer-aided detection, personalized tracking, and monitoring of patients through biosensors use AI, which improves the quality of healthcare systems. This review article provides information about the applications of AI in the pharmacy field along with the benefits and challenges of adopting AI tools.

Introduction

1. Artificial intelligence (AI) is the ability of machine to think like humans and mimics their actions through the simulation of human intelligence [1]. AI influences all the professions across the globe including pharmacy [2]. AI systems have a wide impact on healthcare systems. The manual tasks performed by pharmacists can be replaced with these systems to some extent [3] by decreasing the workload on personnel to integrate and analyse data required for clinical practice [4] This allows researchers to invest their time in the discovery of new drug moieties and novel drug delivery systems. Artificial intelligence improved automation, data-driven decision-making allows to make clinical decisions and overcome problems related to gender bias, and judgemental errors and enhances the usage of novel statistical techniques. R&D divisions of pharmacy industries had introduced small AI teams to focus more on advancements in digital technology based on their scientific priorities [5, 6].

The applications of AI in pharma industries have revolutionized how scientists research new drugs, treat diseases, and more in the previous five years [7, 8]. Artificial intelligence is now been used in pharmaceutical and healthcare industries for a variety of applications including Research and Development, Drug design and discovery, Drug screening, Pharmaceutical product development, prediction of synergism and antagonism, Rare diseases and personalized medicine, individualized treatment and dose regimen in cancer treatment, tracking BMR and real-time digital reporting, fast track dosing and regimen set up, precise medication and drug prescriptions, clinical trial designing, identifying problems in safety and efficacy, clinical diagnosis, patient real-time tracking with wrist sensors,

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predicting outbreaks and treatments, combinatorial medicines, nanorobotics drug delivery systems and so on[1, 9].

Advantages of Artificial Intelligence in the pharmacy sector

1. AI handles large volumes of data with enhanced automation from huge amounts of data [10].
2. Cost and time reduction of clinical trials by constructing cohort studies using AI-based technologies which usually take longer time and are costly [1, 11].
3. Time and expenses involved in the drug discovery process can be reduced and is helpful in recognition of hit and lead compounds [10].
4. AI systems enable automatic data entry through applications like Google's artificial brain [11].
5. To predict the production cost and selection of combination therapy.
6. AI-based systems help in the prediction of physicochemical properties and combination therapy.
7. Artificial intelligence helps to improve the implementation of rational drug designs
8. AI assists in choosing the right therapy for patients i.e., personalized medicine
9. It also helps to manage clinical data for future references in drug developments.
10. Aids in the management and personalized treatment of rare diseases [8].
11. AI was useful to reduce medical errors and improve operational and service quality in hospitals [10].
12. AI provides neural-based guidance in making treatment decisions [11].
13. It is found to be useful in the parallel labeling of data [12].
14. It is also found that AI systems can recognize mutations in DNA and RNA [13].
15. Artificial intelligence helps in dosage error reduction [14].

Disadvantages of application of AI in pharmacy

1. The major concern with these technologies was data challenges and privacy concerns [10].
2. The data is accessed from various data providers which may increase the cost [15].
3. The human source will be reduced so that many will be jobless.
4. Implementation of AI systems in the pharmacy field is difficult due to unfamiliarity and lack of IT infrastructure [8].
5. Implementation is difficult due to ethical issues and the training of personnel [10].
6. System failures are major drawbacks that lead to loss of managerial control and cybersecurity problems [10].

Applications of Artificial Intelligence

Artificial intelligence has spread its wings to many sectors of pharmacy. Few among them are briefly described, they are

1. Research and Development

Using a software-based technology like AI to aid research and development may be quite beneficial. Drug development is being accelerated with the use of computational techniques. These technologies have the potential to tackle challenges in formulation design such as stability, dissolution, porosity, and many others using a quantitative structure-property connection (QSPR) [16].

These systems ensure the development of formulation while cutting down the development period and costs and thus fastening total formulation development procedure. As a result, the use of AI will increase the success rate in the field of research and development [1, 16].

Using the CD3 %, total protein, and patient age as the core feature classification model, researchers discovered four essential medical features that include clinical, laboratory, and demographic information [17].

2. Drug Discovery

The ability of AI to swiftly discriminate between hit and lead compounds, confirm the drug target more quickly and optimize the design of the drug structure might be a benefit to the health sector, reducing the cost and delay involved with the discovery of a novel molecule [1, 10].

Many pharmaceutical corporations have begun to invest in resources, technology, and services to collect and curate data sets to support research in this field, working with software companies to incorporate the most cutting-edge technologies in the costly and time-consuming process of drug discovery [1, 15].

The deep learning technology has progressed from the previous ML approach with the emergence of "big data," and it can now be utilized to cope with the vast number of data created by the whole drug discovery and development chain [1].

Several in-silico methods can be used to predict the chemical structure that will elicit the desired response at the target site, optimize this structure to meet the requirements of various objectives such as potency, safety, solubility, permeability, synthetic tractability, and so on, predict the physicochemical properties of the compound, and plan the compound's synthesis [1, 18].

ML algorithms and software are being developed and used at all stages of drug discovery and development, including clinical trials, to identify novel targets, provide stronger evidence for target-disease associations, improve the small-molecule compound design and optimization, increase understanding of disease mechanisms, increase understanding of disease and non-disease phenotypes, develop new biomarkers for prognosis, progression, and drug efficacy, and improve analytes [19].

For the prediction of druggable targets, physicochemical parameters are used [15]. ML has allowed pharmaceutical companies to access and organize a greater amount of data. Images, textual information, biometrics, and other information from wearables, assay information, and high-dimensional omics data are all examples of data types [15].

AI Tools used in drug discovery are DeepChem, DeepNeuralNetQSAR, DeepTox, Neural Graph Fingerprint, ORGANIC, and Potential net.

3. Role of AI in Target identification and validation

For any newly discovered compound or drug, finding a biological target is critical. At the moment, there are numerous databases on genetic information, making the job difficult to find a target, but through the use of AI, target identification and validation can be performed during clinical trial stages [15].

For breast, pancreatic, and ovarian malignancies, a support vector machine (SVM) classifier was used to identify proteins into drug targets and non-drug targets using multiple genomic data sets. This system identified a slew of cancer targets [20].

Deep learning algorithms were used to compare the performance

of young and old muscles to identify aging biomarkers. Natural language processors, which are an important aspect of AI, are used to mine data from the literature, which is crucial for target validation. [21] Artificial intelligence also plays a prominent role in the identification and designing of targets for small molecules [15].

4. Drug Screening

Researchers have used an AI-driven strategy to link physicochemical factors to molecular descriptors such as atomic charge, hydrogen bonding effects, molecule volumes, and surface area. Lipophilicity can be anticipated using computational methods such as group-contribution (GC) methods, state equations, and conductor-like methods [22].

Screening model (COSMO)/conductor-like screening model for real solvents (COSMO-RS), molecular simulation, and quantum chemistry-driven linear/nonlinear QSPR [22]. Bioactivity prediction using matched molecular pair (MMP) analysis [23]. Predicting the structure of the target protein, as well as drug-protein interactions.

Toxicology prediction is the DeepTox algorithm, which is based on the concept of machine learning and predicts the toxicology of new compounds with high accuracy [24].

Artificial intelligence-based techniques are a great way to explore the intricate simulations and calculations that go into cellular and subcellular protein dynamics. Machine/computer-generated 2° generation compounds could be drug-like candidates for the upcoming 10th generation [1].

Computer-assisted drug design tools have been credited by pharmaceutical companies like Bayer Healthcare and Roche for their recent success in producing improved pharmacophores.

When compared to their respective training sets, the distributions of molecular weight, estimated logP, number of hydrogen bond acceptors and donors, number of rotatable bonds, and topological polar surface area [25]. Alpha Fold, for example, uses simple protein main sequences as inputs to predict the target protein's 3D structure using a complicated algorithm based on deep neural network fundamentals (DNNs) [25].

Models for drug screening

To predict physicochemical features with the use of AI-novel generated anticancer medicinal compounds, researchers used the ResNet convolutional neural network architecture [26].

Deep learning prediction of solubility showed better results than standard solubility techniques when using a recursive neural network for the prediction of properties like aqueous solubility [27].

To predict the biological activity of manufactured chemicals using AI, an adversarial auto-encoder with entangled conditions was developed. Following the application of the AI model, a few compounds having drug-gable features were found and examined in-vitro for biological activity to identify prospective Janus kinase 3 inhibitors. Few compounds exhibit particular target bioactivity against the target [28].

To test the antibacterial potential of the essential oils, a fast artificial neural network (FANN) was employed. In addition, the applied model predicts two to three bioactivities at the same time. The researchers found that FANN is a quick, low-cost, and accurate approach for predicting antimicrobial activity [28].

eToxPred Molecular toxicity prediction of natural synthesized and recognized pharmaceuticals, as well as dangerous chemicals The researchers of this work used machine learning algorithms that works on the molecular fingerprints to screen substances in algorithms [29].

Toxicity prediction using DeepTox based on a protein-ligand interaction study Deep learning outperforms classic computational toxicity prediction methods such as naive Bayes, random forests, and support vector machines in predicting toxicity, according to the researchers [30].

They used a machine learning approach called GENTRL to locate effective inhibitors of the discoidin domain receptor 1 (DDR1) after creating DDR1 inhibitors and produced six leads that met the Lipinski rule of five. After that, biochemical testing was carried out, which revealed that four of the six compounds were active, two of which were verified in cell-based assays, and one lead was examined in preclinical animal investigations to establish a pharmacokinetic profile [31].

Design of pharmaceuticals API EPE neural network algorithm has been modified (NN) Predicting the structure of secondary proteins The neural network's ability to extract power from the protein structure CB513 database and determine the structure of the targeted protein was explored by the researchers [32].

Design of pharmaceuticals to find drug-protein target interactions, a convolutional neural network (CNN) was used. The researchers claimed that the novel model can predict drug-target interactions more accurately than traditional methods [33].

Neural computers with adversarial threshold (ATNC) De-novo tiny organic molecules were created for a design. The researchers compared the ATNC and the ORGANIC models to identify the best medication. ATNC elicited stronger drug-likeness qualities with greater precision than ORGANIC. De novo AI is a method for discovering novel active compounds for hit-to-lead identification [34].

5. Prescription

As we are familiar with after diagnosis of a disease, a prescription was prepared which contains the list of medicine that is to be consumed by the patient. The job of prescribing medicines was generally the role of the physician, which is sometimes prone to prescription errors. To minimize prescription errors, AI has come up with AI-based knowledge bots which prevent toxic effects caused due to prescription errors [1].

Knowledge bots based on AI can be used in medical diagnosis for a variety of clinical diseases. For patients or clients, a personalized self-service adviser will provide similar counsel and support as would be provided by the world's greatest specialists. These AI bots will both retrieve and communicate patient information to a third-party pharmacy. Furthermore, depending on the patient's whole medical history, these AI bots will offer the best medication for the patient, which they will then review and validate [1, 35].

6. Pharmaceutical product development

Expert systems can be useful as efficient decision-making tools in the development of medicinal products. These expert systems can be used to choose the type and amount of excipients for tablet and capsule formulation [36].

Systemic toxicity, restricted therapeutic index, and dose modification in prolonged therapy are some of the issues connected with traditional and regulated drug delivery systems that can be conquered with the aid of artificial intelligence [1].

The process of developing pharmaceutical products is a multivariate optimization issue. The capacity of artificial neural networks to generalize is one of their most valuable qualities. These characteristics make them ideal for tackling formulation optimization difficulties in pharmaceutical product development. In research on the influence of numerous elements on tablet qualities, Artificial neural network (ANN)

models revealed greater fitting and forecasting abilities in the production of solid dosage forms (such as dissolution). ANNs proved to be a beneficial tool for developing micro-emulsion-based medication delivery systems with minimal experimental effort [37].

Some of the AI-based systems employed in pharmaceutical product management are the Usage of microchips in the treatment of diabetes, Nano-robots, Controlled insulin delivery, Nano-medicine, and Combination drug delivery [1].

7. Synergism and antagonism

In a therapeutic intervention, identifying and analyzing drug synergism and antagonism is critical because it aids in dose reduction and toxic and side effects of combinational medications are avoided. The master regulator inference algorithm (MARINA) is used by SnuGen to forecast synergism and antagonism. Choosing input parameters is a critical issue when utilizing AI for combination therapy [1, 38].

8. Clinical diagnosis and treatment

AI-based systems have an impact on the clinical diagnosis and treatment of several diseases. Clinical diagnosis for disorders such as heart disease, stroke, pancreatic cancer, diabetic nephropathy, and bladder cancer improved from AI interventions. In dermatology, artificial intelligence (AI) is viewed as a potential method for diagnosing and identifying skin lesions [1].

Image processing, computer vision, ANN, ML, CNN, and deep learning are some of the AI technologies that can be utilized in the medical field. Image processing is a mathematical method for improving image quality, pattern recognition, and pattern measurements which is helpful in diagnosis [1]. Computer-aided diagnostics, image-guided surgery, and virtual colonoscopy are just a few of the applications for axial imaging [12].

Radiology, pathology, dermatology, and ophthalmology, all of which rely on imaging data, have already begun to reap the benefits of AI applications [13]. Deep Learning (DL) can also be used to reduce the quantity of radiation used in computed tomography (CT) imaging or to speed up the acquisition of magnetic resonance imaging (MRI) data [15].

AI-based systems such as machine learning (ML) and Natural language processing (NLP) aims to discover precise medicines in the treatment of serious illness such as cancer by monitoring changes in tumors [39].

MYCIN was established to use 450 guidelines gathered by a medical professional to cure bacterial illnesses by advising people on the best drugs to take. This type of expert system assists doctors and medical specialists with clinical decision-making [40].

Many fields with big data components, such as DNA and RNA sequencing data processing, are predicted to gain from AI [13]. Foundation Medicine and Flatison health by Roche focuses on cancer diagnosis and therapy suggestions based on genetic profiles [15, 39] and knowing genetic changes in Alzheimer's disease [15]. Some AI tools were also developed to detect epilepsy [41].

Machine learning models for community health to identify populations at risk of specific diseases or accidents, as well as to predict hospital readmission. Across the care continuum, machine learning and business rules engines are increasingly being employed to develop complicated treatments [1]. Usage of computer-aided detection (CADe) in clinical use has been proposed and utilized occasionally [13].

The combination of search engines like google and AI-based systems provides image searches from a huge amount of data which is useful in clinical diagnosis. Google also tied up with health delivery systems for building big data prediction models to alert physicians regarding high-risk illnesses like heart failure [1].

A potential subject of research is messaging notifications and relevant, targeted content that prompts actions at critical phases. Health trackers like Fitbit, and Apple also monitor heart rate, activity, and sleep levels [11]. Online therapy of AI was also developed to reduce social anxiety as a treatment aid for cognitively impaired patients [11].

Many AI-based medical applications are already in use, ranging from online appointment scheduling, online check-ins in medical centers, digitization of medical records, reminder calls for follow-up appointments, and immunization rates for children and pregnant women to drug dosage algorithms and adverse effect warnings when prescribing multidrug combinations [11].

The recent ongoing research on AI and ML-based systems shows better tools for diagnosis, treatment, contact tracing, and vaccine development in the case of COVID19 which minimizes the human intervention and yields accurate results in less time. Drugs like chloroquine are found to be effective in the case of COVID19 treatment was founded by researchers through the development of models based on AI tools [40].

Various afflicted nations develop a mobile application that uses technologies such as Bluetooth, GPS, Social graphs, contact details, network-based API, mobile tracking data, card transaction data, and system physical address to create a digital contact tracing process. The digital contact tracing technique can function in virtually real-time and at a much faster pace than a non-digital system. All of these digital apps are designed to collect specific personal data, which will be analyzed by machine learning and artificial intelligence (AI) algorithms to locate a person who is vulnerable to a particular virus due to their recent contact chain [40].

9. Clinical trial design

As the number of clinical trials grows, finding novel biomarkers to identify people who respond to a specific treatment will become more crucial. Availability of huge information regarding computational pathology, which enables the discovery of new biomarkers and their generation in a more exact, repeatable, and high-throughput manner, would shorten the time for drug development and provide faster treatment to the patients [15].

Thousands of publications on biomarkers and predictive models have been published, but only a few have been employed in clinical trials. Data quality, model selection, data, and software availability, model repeatability, and the design of clinically relevant tests are all factors that contribute to the gap. Several community initiatives have looked into using machine learning approaches to build classification and regression modelstoo tackle some of the model-related problems [15, 42].

Regression analysis methods, which are more appropriate than manual analysis, can be used to identify risk-based genes. The US Food and Drug Administration has authorized just a few models for predicting clinical outcomes using baseline gene expression data [43].

Machine learning-based predictive biomarkers in non-oncology indications, such as rheumatoid arthritis, BMI calculation, coronary artery disease, atrial fibrillation, type 2 diabetes, inflammatory bowel disease, and breast cancer, have made substantial progress utilizing diverse forms of input data. Target validation, the discovery of prognostic biomarkers, and the analysis of digital pathology data are all examples of clinical research. [15].

10. Personalized medicine

These approaches are also employed in medicine, and when paired with pharmaceutical development, they might lead to substantial advances in personalized treatment. ML has also been used to integrate electronic health records and real-world information to enhance clinical trial results and optimize the process of clinical trial eligibility screening [1, 15].

Using AI-based methods, the pharmaceutical industry is focusing on pd4 inhibitors to pinpoint drugs used in the treatment of rheumatoid arthritis [25].

Challenges

The major challenges involved in adapting AI in pharmacy are

1. Complexity of the technology
2. Lack of trust due to privacy errors
3. It is very difficult to adapt deep learning algorithms in practice currently.

Conclusion:

Humans are rigorously trying to develop systems that mimic human intelligence. AI is the most satisfying system that performs tasks like humans. AI is expanded to pharmacy and healthcare systems by replacing traditional methods with more advanced techniques, which decreases time and costs. AI focuses on generating real-time, evidence-based support in decision-making in every division of pharmacy, from research to prescription and patient tracking.

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Conflict of Interest

The author(s) confirm that this article content has no conflict of interest.

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