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Revolutionizing Healthcare: AI in Drug Discovery and Pharmacy Practices

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Abstract

Artificial intelligence (AI) has emerged as a revolutionary element across numerous sectors, especially in healthcare and pharmacy. AI systems that can execute functions typically necessitating human intelligence, such as learning, problem-solving, and speech recognition, are poised to transform drug discovery, enhance patient care, and reshape pharmacy practices. AI can help discover drugs with predicting interactions with drug destinations, virtual screening, drug reuse, and drugs that accelerate the development of effective treatments. AI also contributes to clinical research by optimizing patient recruitment and research design. In pharmacy practices, AI improves individuality medicine, clinical decision support, drug therapy compliance and drug-specific surveillance. The benefits of AI include increased accuracy, increased efficiency, and personalized treatment plans, but challenges such as data integration and algorithmic transparency remain. The future of AI in pharmacies is promising. Continuous advancements are presented to revolutionize patient care and health systems, making them more efficient and cheaper, supporting clinical decision-making, medication adherence, and pharmacovirality.

Keywords: Artificial intelligence, drug discovery, pharmacy practice, personalized medicine, clinical decision support, medication adherence, pharmacovigilance

INTRODUCTION

Artificial intelligence (AI) is a subset of computer science dedicated to developing intelligent systems capable of executing tasks that typically demand human cognitive abilities. These tasks include discussion, learning, problem-solving, language recognition, and understanding. In the field of pharmacy, AI has become a transformative force, providing advanced solutions in drug discovery, clinical decision support, personalized medicine, and patient safety. With the increasing complexity of drug development and healthcare systems, AI is playing an essential role in enhancing efficiency, accuracy, and outcomes [1-4].

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The aim of this review is to discuss how AI is reshaping drug discovery processes, improving patient care, and transforming pharmacy practice. We will delve into the application of AI in various stages of drug development, including target identification, drug screening, clinical trials, and post-market surveillance, as well as its role in clinical pharmacy and patient monitoring [5–8].

CLASSIFICATION OF ARTIFICIAL INTELLIGENCE (AI)

AI can be classified in two different ways [9, 10]:

a. According to caliber; and
b. According to the presence (Table 1).

Table 1. Classification of AI.

Based on the Caliber	Weak Intelligence, Artificial Narrow Intelligence, Artificial general Intelligence, and Artificial Super Intelligence
Based on presence	Type 1: reactive machine. Type 2: limited memory system. Type 3: based on the theory of mind. Type 4: self-awareness.

AI According to Caliber

Weak Intelligence or Artificial Close Intelligence (ANI)

Weak Intelligence, also known as Artificial Narrow Intelligence (ANI), is a type of AI that:

- Excels at one specific task.
- *Is trained to perform a narrow function, such as:*
  - Recognizing faces.
  - Driving a car.
  - Playing chess – Translating languages.

Artificial General Information (AGI) or Powerful AI

Also known as human level AI. It simplifies human intellectual skills. This allows you to find a solution if you are exposed to unknown tasks. AGI can do everything as a human being [11].

Artificial Super Intelligence (ASI)

A more active brain power than intelligent people in pictures, mathematics, space, etc. In all fields, from science to art. It is not within the range of signs that are smarter than humans.

AI according to Presence

There are three types of AI systems:

Type 1. Reactive Machines

These AI systems can only react to current situations. They do not have memories or learn from past experiences. Examples include:

- Deep Blue, a chess program that beat the world champion.
- Google's AlphaGo, a program that plays the game Go.

Type 2. Limited Memory

These AI systems can use past experiences to make decisions. They can learn from data and improve over time. Examples include:

- Self-driving cars that use past observations to make decisions.
- Virtual assistants that learn your preferences over time.

Type 3. Theory of Mind

This type of AI system does not exist yet. It would be able to understand human thoughts, intentions, and emotions, and use that understanding to make decisions.

Type 4. Self-Aware AI

These AI systems are still in the realm of science fiction. They would have:

- *A sense of self:* They would know they exist and have their own identity.
- *Consciousness:* They would be aware of their own thoughts, emotions, and experiences. If a machine has self-devotion, it understands the state and uses ideas that exist in other people's brains. This is an AI that does not exist.

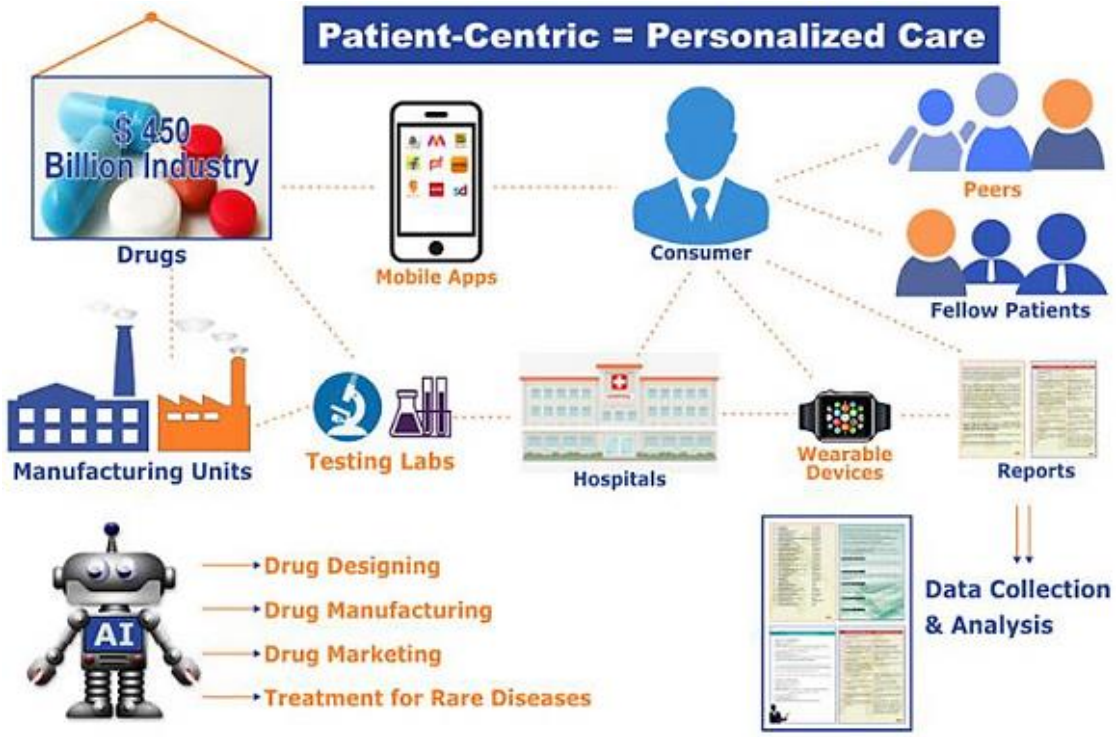

Figure 1. Benefits of using artificial intelligence for drug development.

Table 2. List of important AI-based computer-assisted tools used in drug discovery.

AI-Based Computer-Assisted Tools Used in Drug Discovery	Websites	Descriptions
Chemputer	https://zenodo.org/record/1481731	More standardized set-up for reporting chemical synthesis.
ODDT	https://github.com/oddt/oddt	For use in chemo informatics and molecular modelling.
ORGANIC	https://github.com/aspuru-guzik-group/ORGANIC	Molecular generation tool to create molecules with desired characteristics.
DeepChem	https://github.com/deepchem/deepchem	A python-based AI tool for drug discovery predictions.
DeepNeuralNet-QSAR	https://github.com/Merck/DeepNeuralNet-QSAR	Predictions of molecular activity.
Neural Graph Fingerprints	https://github.com/HIPS/neural-fingerprint	Property prediction of novel molecules.
Hit Dexter	http://hitdexter2.zbh.uni-hamburg.de	Machine learning models for the prediction of molecules, which might respond to biochemical assays.
NNScore	http://rocce-vm0.ucsd.edu/data/sw/hosted/nnscore/	Analysis of neural network-based scoring function for protein-ligand interactions.
DeepTox	www.bioinf.jku.at/research/DeepTox	Prediction of toxicity and biocompatibility.
PotentialNet	https://pubs.acs.org/doi/full/10.1021/ acscentsci.8b00507	Ligand-binding affinity prediction based on a graph convolutional neural network.
REINVENT	https://github.com/MarcusOlivecrona/REINVENT	Molecular *de novo* design using RNN and reinforcement learning.
DeltaVina	https://github.com/chengwang88/deltavina	A scoring function for rescoring protein-ligand binding affinity.
AlphaFold	https://deepmind.com/blog/alphafold	Prediction of protein 3D structure prediction.

AI IN DRUG DISCOVERY

1. *Drug Target Identification and Validation:* The early stages of drug discovery often involve identifying suitable biological targets that can be modulated to treat specific diseases. AI can quickly analyze large amounts of biological data, such as genetic information, to find new targets for medicines. By using machine learning, AI can spot patterns and connections in the data that humans might miss. For example, AI-based systems have been used to identify novel drug targets for diseases such as cancer, Alzheimer's, and cardiovascular conditions (Table 2] [1–9].
2. *Virtual Screening and Drug Repurposing:* Traditional drug screening is – consuming and resource – intensive, often requiring the testing of thousands of compounds. AI technologies, particularly machine learning and deep learning models, are being used to predict the biological activity of chemical compounds and screen large libraries of molecules virtually. AI is helpful in finding new uses for existing medicines. It can identify drugs that might work for different diseases and speed up the development of new treatments for emerging diseases.
3. *Predicting Drug-Drug Interactions (DDIs):* Drug-drug interactions (DDIs) can lead to serious adverse effects, complicating treatment regimens. AI systems are being used to predict potential DDIs by analyzing existing clinical and pharmacological data. Machine learning algorithms can analyze chemical structures, pharmacokinetics, and molecular interactions to predict how different drugs may interact in the human body. This ability is crucial for improving patient safety and optimizing drug prescriptions [3].
4. *Clinical trials in AI:* AI plays a critical role in designing and performing clinical research. Traditionally, clinical trials are costly and often fail to deliver results due to patient recruitment challenges, non-response, or high dropout rates. AI-based tools are improving patient recruitment by identifying eligible candidates through the analysis of electronic health records (EHRs). Additionally, AI models are used to optimize trial designs, predict patient responses, and analyze complex trial data more efficiently, thus enhancing the probability of success and reducing the time to market [4].

AI IN PATIENT CARE AND PHARMACY PRACTICE

1. *Personalized Medicine:* One of the most promising applications of AI in pharmacy is the advancement of personalized or precision medicine. AI systems use a patient's unique information, such as their genes, medical history, and daily habits, to suggest personalized treatment plans. By analyzing large datasets, AI algorithms can help predict how a patient will respond to a specific medication, enabling pharmacists to tailor drug therapies to optimize efficacy and minimize side effects [5]. This personalized approach is particularly relevant in oncology, where AI is used to predict treatment responses in cancer patients based on genetic mutations and tumor profiles.
2. *Clinical Decision Support System (CDS):* More and more pharmacies are using computer systems that rely on AI to help pharmacists make better decisions about patient care. These systems assist pharmacists in making clinical decisions by providing evidence-based recommendations, alerts for potential drug interactions, dosage adjustments, and guidance on therapeutic alternatives. By leveraging machine learning algorithms, CDSS can continuously update its recommendations based on new evidence, ensuring that pharmacists have access to the most current information [6].
3. *Medication Adherence Monitoring:* Ensuring that patients adhere to prescribed medication regimens is a key challenge in pharmacy practice. AI technologies are being used to monitor medication adherence using mobile health applications, wearable devices, and AI-driven platforms. For instance, AI systems that use facial recognition or voice recognition technology can verify that patients are taking their medications as prescribed, thus improving medication compliance and patient outcomes [7].
4. *Pharmacovigilance and Drug Safety:* AI is enhancing the monitoring of drug safety by analyzing large volumes of adverse event data collected from healthcare providers, patients, and regulatory agencies.
5. Pharmacy practice: Algorithms for Natural Language Processing (NLP) and Machine Learning provide relevant information from unstructured data sources such as medical documents and social media posts to identify potential concerns about drug safety can be extracted. AI tools are capable of detecting signals of adverse reactions earlier than traditional methods, enabling faster responses from regulatory bodies and pharmaceutical companies [8].

BENEFITS OF AI TECHNOLOGY

The potential benefits of AI technology are (Figure 1) [10–12]:

i. *Accuracy:* Intelligent robots are made of resistant metal bodies and can withstand aggressive air spaces. Therefore, they are sent to explore the room.
ii. *Difficult Exploration:* AI demonstrates its usefulness in mining areas. It is also used in the fuel exploration department. AI systems can examine the ocean by defeating mistakes caused by humans.
iii. *Everyday Applications:* AI is extremely useful in our daily lives, making various tasks and activities more efficient and convenient. For example, GPS systems are primarily used for long drives. Installing AI on Androids can help you predict what people type. It also helps you fix spelling errors.
iv. *Digital Assistants:* Many organizations use AI-powered digital assistants, like avatars, to help with tasks. These assistants make logical decisions without being influenced by emotions, making them efficient.
v. *Repetitive Tasks:* Humans can only do a few tasks at a time, but machines can handle many tasks simultaneously. Machines can also analyze information faster and more accurately than humans. Plus, you can adjust machine settings, like speed and time, to meet your needs.
vi. *Medical Use:* Generally, physicians can assess a patient's condition and analyze other health risks related to drugs with the help of AI programs. Apprenticeships from applications of AI programs such as various simulators for artificial surgery (e.g. gastrointestinal intestines – simulation, heart simulation, brain simulation, etc.
vii. Work for long hours without confusion or boredom.
viii. *Growth rate:* AI technology is often used in the most advanced technological innovations around the world. You can create a variety of computer modeling programs and aim to invent new molecules. AI is also used to develop new medicines and treatments, leading to breakthroughs in healthcare.
ix. *No risk:* When working in dangerous zones such as fire stations, there is a great opportunity to injure dedicated personnel. Machine learning programs can be repaired in the event of misfortune.
x. *Functions like AIDS:* AI technology served different functions by operating children on a 24/7 basis and operating the oldest. It can serve as a source of education and learning for all.
xi. *Borderless functions:* Machines are not limited to limits. A machine without emotions can do everything efficiently and produce more accurately than humans

LIMITATIONS AND DRAWBACKS OF AI TECHNOLOGY

The important drawbacks of AI technology are [13, 14]:

i. Intricate design, maintenance and repair of machines is very inexpensive. Designing an AI machine requires a long period of time. AI machines must regularly update their software programs. New installations and repairs of machines will consume a lot of time and a lot of money.
ii. *Non-replica person:* robots with AI technology add some advantages to performing given tasks without evaluation, so they are not human or emotional in the sense that they have no human or emotional thinking. It is associated with force. If an unknown problem occurs, the robot cannot make decisions and give false reports.
iii. *Lack of experiential improvement:* Unlike HR departments, which can refine their processes through experience, AI-powered machines do not learn from experience. Additionally, it is challenging to distinguish between high-performing and underperforming individuals, as AI systems process information uniformly, without personal biases or subjective evaluations.
iv. *Limited creativity:* AI-powered machines lack emotional intelligence, sensitivity, and original creativity. Humans possess unique abilities to perceive, think, and feel, enabling them to generate

innovative ideas and solutions. In contrast, machines, no matter how advanced, cannot replicate the depth and complexity of human creativity.

v. *Job loss and unemployment:* The rapid integration of AI technology across multiple sectors poses a significant threat of widespread unemployment, as automation replaces human workers, potentially displacing millions of jobs. Unwanted unemployment can lead to human workers losing their work habits and creativity.

CHALLENGES AND FUTURE DIRECTIONS

One of the main concerns is integrating AI technology into existing health infrastructure. Many health systems lack the required data exchange framework, which can limit the effectiveness of AI control solutions. Furthermore, there is concern about the transparency and interpretability of AI algorithms, especially when used in clinical decision making.

It is essential to explain and be trusted to provide medical service providers and patient acceptance. The ability to analyze complex data records, predict results, and optimize treatment plans is promising in improving healthcare efficiency, accuracy and personalization. Since the adoption of AI continues to expand, the pharmaceutical industry must actively tackle the challenges associated with integration. AI has the potential to transform pharmacies, leading to better patient care, improved health outcomes, and a more efficient healthcare system, but it requires a thoughtful and strategic approach. The future of AI in pharmacy is promising, with ongoing advancements in AI algorithms, data collection, and integration technologies. As AI systems become more sophisticated, their potential to improve patient care, optimize drug development processes, and reduce healthcare costs will only increase. Researchers, healthcare providers, and policymakers must work together to overcome the challenges associated with AI implementation and ensure that its benefits are accessible to all.

CONCLUSIONS

AI has the potential to turn every aspect of pharmacy care from drug detection to clinical care and patient monitoring. The ability to analyze complex data records, predict results, and optimize treatment plans is promising in improving healthcare efficiency, accuracy and personalization. Since the adoption of AI continues to expand, the pharmaceutical industry must actively tackle the challenges associated with integration. By leveraging AI effectively, pharmacies can experience a transformative shift, leading to enhanced patient outcomes, improved operational efficiency, and a significant reduction in healthcare costs.

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