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REVIEW

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Emerging of artificial intelligence and technology in pharmaceuticals: review

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Abstract

Background The review covers a variety of Artificial intelligence (AI) related topics in medication development. Additionally, it gives a quick account of the recent advances made in drug development by the pharmaceutical industry in cooperation with various AI. All facts of science have been impacted by advances in computing and technology. In all fields of science and technology, from fundamental engineering to medicine, AI has become a crucial component. AI has so influenced pharmaceutical chemistry and health care.

Main body The use of computers to assist in drug creation has overtaken more conventional approaches in recent years. AI is frequently utilised to reduce the amount of time and improve drug design processes. The success rate of the developed medicine is further increased by the ease with which the target proteins may be discovered utilising AI. Every step of the medication design process involves the use of AI technology, which lowers the cost and greatly lowers the health hazards related to preclinical studies. AI is a powerful data mining technique that is based on vast amounts of pharmaceutical data and the machine learning process.

Conclusion The use of AI in de novo drug design, activity scoring, virtual screening, and In silico evaluation of drug molecule characteristics is the consequence (absorption, distribution, metabolism, excretion, and toxicity). To speed up drug research and the healthcare system, pharmaceutical companies have joined with AI firms.

Keywords Artificial intelligence, Drug design, Pharmaceuticals, Artificial neural network, Quality by design, Technology

Background

A key component of intelligence is the capacity for logical reasoning, which has long been the main area of AI study. A theorem-proving program created in 1955–1956 by Allen Newell, J. Clifford Shaw, and Herbert Simon of the RAND Corporation and Carnegie Mellon University is regarded as a significant milestone in this field. The ability of a digital computer or robot controlled by a computer to carry out tasks typically accomplished by intelligent beings is known as AI [1]. The phrase is frequently used in the quest to develop AI systems with cognitive capabilities resembling those of humans, such as the ability to reason, find meaning, generalise, and learn from experience. It has been established since the 1940s, when the first digital computers were developed, that computers can be programmed to carry out incredibly challenging jobs [2].

Today's pharmaceutical market accepts medications after a lengthy and costly drug development process. The majority of drugs cost billions of dollars and take 10 years or more to reach the pharmaceutical market. This requires more money and more time for drug

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development. The concept of AI appears to be more promising in overcoming these drawbacks and should result in successful drug development programs [3]. AI is being used in new technologies such as drugs, prosthetics, and evolving and advanced robotics. Additional benefits of AI in the drug development process include identifying drug targets, suggesting molecules from data libraries with chemical modifications, and sometimes repurposing the drug [4].

Main body

As it is evident, current developments in AI have led to the development of a number of technologies that could be used in the creation of pharmaceutical products. Those who can take and utilise this technology as a tactical weapon will be the "winners" in a period of escalating rivalry. Turning potential into action is difficult because there is a chance to boost productivity while also enhancing consistency and quality where applications have succeeded [5] (Fig. 1).

AI goals

- *Expert system development*: It involves creating automated systems that operate intelligently and counsel people on how to proceed.
- *Human intelligence in computers*: It will assist in the development of analogous cognitive patterns in computers, enabling them to behave like people and take the necessary measures to resolve challenging situations.
- *Multi-domain applications*: AI will aid in the implementation of multiple domains such as psychology, medical science, ethics, natural sciences, healthcare, and more [6].

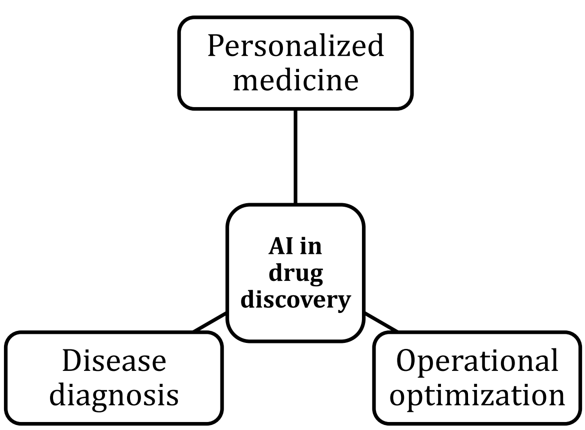

Fig. 1 Trends in AI

Literature review

In a study, model trees, a form of AI, were used to model a database of formulations for immediate-release tablets. Artificial neural networks, which are well-known and frequently used in the disciplines of pharmaceutical product formulation, were utilised to compare the model's performance to those networks. The correlation coefficient (R^2) was used to evaluate the derived models predictability. Similar in quality to neural network models, multivariate linear equations derived from model tree studies were able to predict tablet tensile strength, disintegration time, and drug dissolution profiles. However, these equations uncovered additional, important data that had been kept secret in the formulation database. Model trees, as a transparent technology, are concluded to be useful tools for formulators [7].

By analysing the chemical structures of kinases, the author was able to determine their polypharmacology using KinomeX, an AI-based online platform based on Deep neural neutrons (DNNs). The DNN used by this platform was trained on 14,000 bioactivity data points obtained from more than 300 kinases. Therefore, it has real-world implications in determining a drug's general selectivity towards the kinase family and particular kinase subfamilies, aiding in the development of various modifiers. One notable example is Ligand Express, Cyclica's cloud-based proteome-screening AI technology. Finding receptors that can have both onand off-target interactions with a certain small chemical is done using this method. This facilitates comprehension of the medication's potential negative effects [8].

AI's ability to predict drug-target interactions has also been used to avoid polypharmacology and aid in the repurposing of medications. A medication that has been repurposed is eligible for Phase II clinical trials right away. This lowers spending as well because relaunching an existing medicine is less expensive ($8.4 million) than introducing a brand-new pharmacological entity ($41.3 million). It is possible to predict the novel relationship between a drug and an illness using the "guilt by association" technique, which is either knowledge-based or computationally driven. The Machine learning (ML) approach which makes use of methods like Support vector Machine (SVM), Neural network (NN), logistic regression, and Deep learning (DL) is popular in networks that are computationally driven. When repurposing a medicine, ML techniques like PREDICT, SPACE and logistic regression platforms take a drug's gene expression profile into account [9].

The basic concept of AI in pharmaceutics

There are two major categories for AI developments. The first group includes technological methods and software, such as expert systems, that imitate human experience and draw conclusions from a set of rules. Devices that mimic how the brain operates, such as artificial neural networks, fall under the second group artificial neural network (ANNs). The ability of artificial neural networks to generalize is one of their most advantageous traits. These characteristics make them excellent for dealing with issues relating to formulation optimization in the development of pharmaceutical products [10] (Table 1).

How does AI works

Building an AI system involves carefully replicating human characteristics and skills in a machine and using that machine's processing power to outperform our talents. Understanding the different sub-domains of AI and how they could be applied to different fields of the industry requires a deep dive into the subject.

- *Machine learning (ML)*: ML teaches a computer how to draw conclusions and make decisions based on prior knowledge. Without relying on human experience, it recognizes patterns and examines historical data to deduce the significance of these data points and arrive at a potential conclusion [20].
- *Deep learning (DL)*: A machine learning technique is deep learning. DL rejuvenated neural network in 2000s which trained deeper networks. To classify, infer, and forecast the outcome, it teaches a machine to interpret inputs through layers. For example, it helps in knowing the complex internal representation which are necessary in understanding the difficult language or analyzing the objects by a way of going through in depth layers of activity vectors and finding the connection strengths that motivates these vectors by knowing stochastic gradient [21].
- *Neural networks (NN)* These systems operate in a manner akin to human neural cells. They are a group of algorithms that mimic the way the human brain works by capturing the relationship between numerous underlying variables [17].
- A machine's ability to read, comprehend, and interpret a language is known as Natural language processing (NLP). A computer will react appropriately once it recognizes the user's intended message [15].
- *Computer vision*: By dissecting an image and examining various aspects of the item, computer vision algorithms attempt to comprehend an image. This aids the machine in classifying and learning from a collection of photos, enabling it to produce superior results based on prior observations [11].
- *Cognitive computing*: By analyzing text, audio, images, and other inputs in the same way that humans do, cognitive computing algorithms attempt to simulate the functioning of the human brain and provide the desired results. Additionally, enrol in free courses on AI applications [16] (Fig. 2).

Table 1 List of AI-based computational tools for drug delivery

Tools	Description	Website URL	References
Alpha fold	Protein 3D structure prediction	https://deepmind.com/blog/alphafold	[10]
Chemputer	A more standardized format for reporting a chemical synthesis procedure	https://zenodo.org/record/1481731	[11]
DeepChem	A python-based AI tool for various drug delivery task predictions	https://github.com/deepchem/deepchem	[12]
Deep neural net-QSAR	Molecular activity predictions	https://github.com/Merck/DeepNeuralNet-QSAR	[13]
Deep tox	Toxicity predictions	www.bioinf.jku.at/research/DeepTox	[14]
Delta vina	A scoring function for rescoring protein–ligand binding affinity	https://github.com/chengwang88/deltavia	[15]
Hit dexter	ML models for the prediction of molecules that might respond to biochemical assays	http://hitdexter2.zbh.uni-hamburg.de	[16]
Neural graph fingerprints	Property prediction of novel molecules	https://github.com/HIPS/neural-fingerprint	[17]
NNScore	Neural network-based scoring function for protein–ligand interaction	https://pubs.acs.org/doi/full/10.1021/acscentsci.8b00507	[18]
ODDT	A comprehensive toolkit for use in chemoinformatics and molecular modeling	https://github.com/aspuru-guzik-group/ORGANIC	[19]

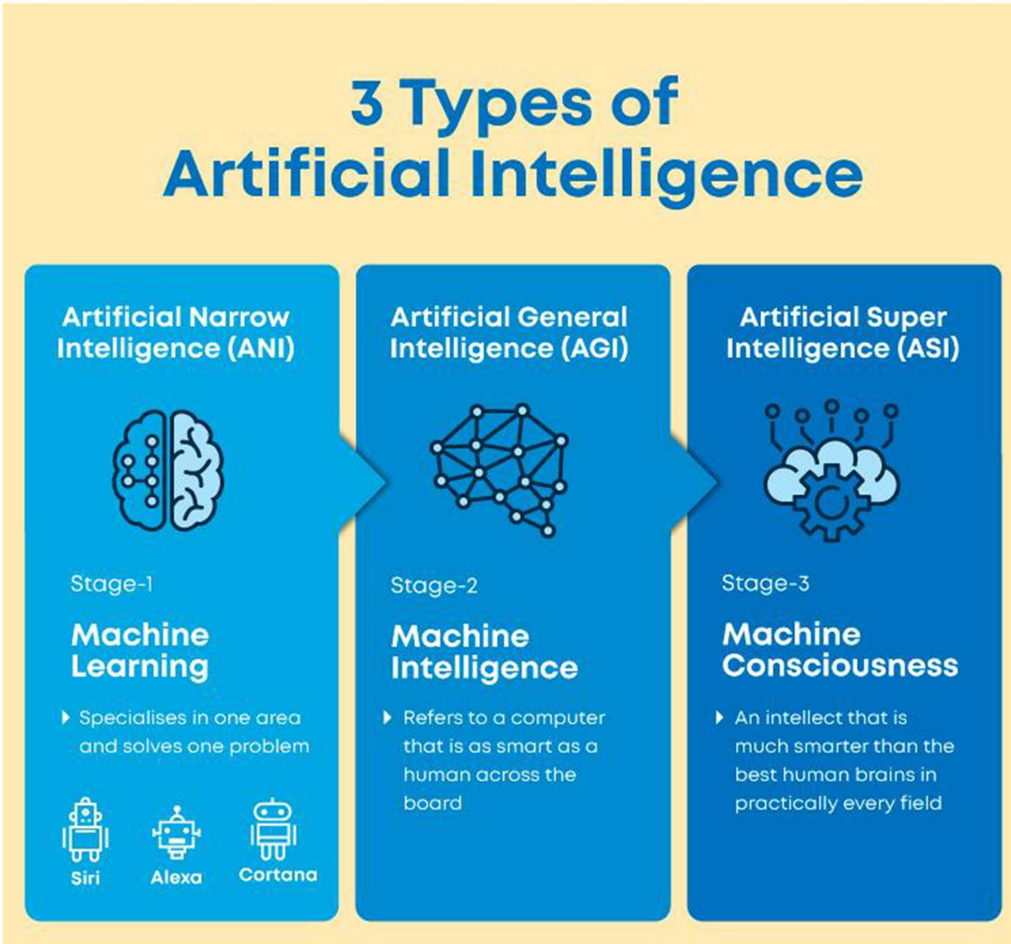

Fig. 2 3 Types of AI

Applications of AI in pharmaceuticals and drug delivery

The power of long-term learning is often removed after training when an AI system is employed to regulate processes like manufacturing or clinical trials. The pharmaceutical industry has improved since the relatively recent adoption of Quality by design (QbD) methodologies, nevertheless, and the latest industry 4.0 initiatives seems to portray a sector in rapid development [22]. Therefore, there is a strong likelihood that if an early AI application is developed, it will be put into use. In contrast to other scientific fields, pharmaceutical sciences can cause delays in data codification and standardisation. Data accumulation and standardisation are essential for effectively training AI in the former [23] (Fig. 3).

AI used

The following are some examples of how AI is used in data processing:

1. Data searching and search engine optimization to produce the most pertinent results.
2. If–then logic chains that can be used to carry out a series of instructions dependent on parameters.
3. Pattern detection to find noteworthy patterns in vast data sets for original insights
4. Using probabilistic models to anticipate future results [24].

AI in health care

- *Administration*: AI systems are assisting with daily administrative activities to minimize human mistakes and maximize productivity. Natural language processing (NLP) transcriptions of medical notes help organize patient information so that clinicians can read it more easily.

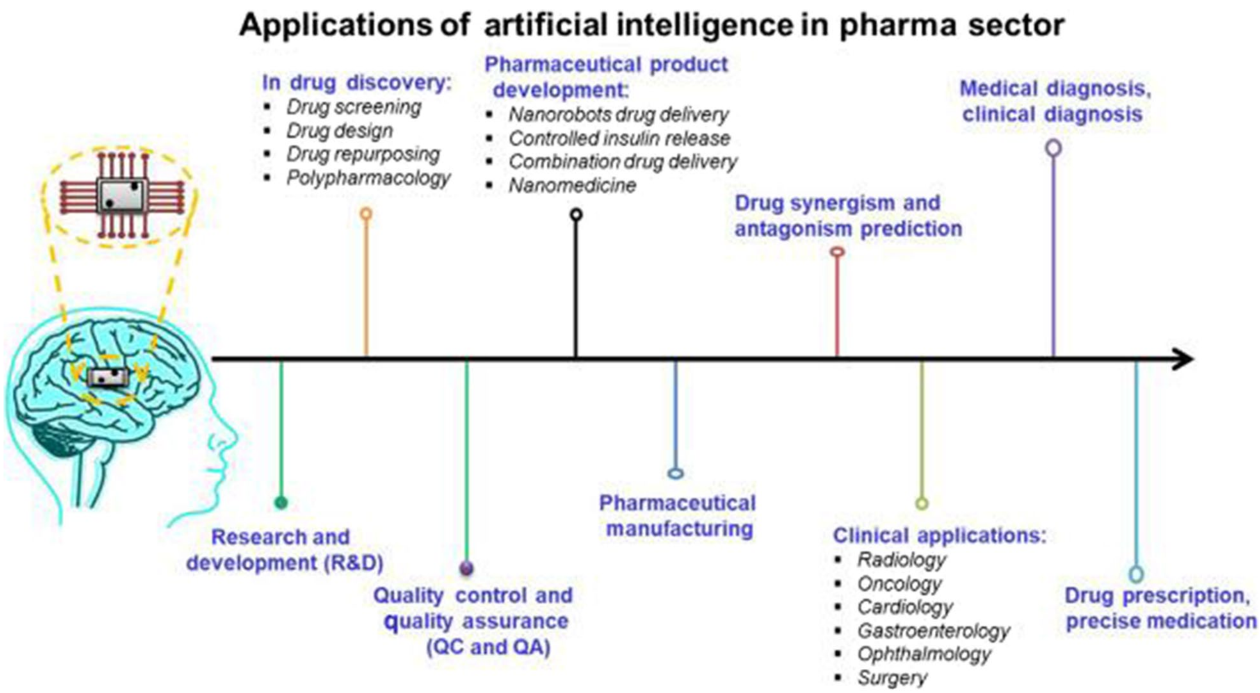

Fig. 3 Applications of AI in the pharma sector

- *Telemedicine*: In non-emergency scenarios, patients can contact a hospital's AI system to analyze their symptoms, enter their vital signs, and determine whether they require medical assistance. Giving them only the most urgent situations lessen the workload of medical experts.
- *Assisted diagnosis*: AI is now capable of reading MRI scans to look for tumors and other malignant growths at an exponentially faster rate than radiologists can, with a significantly narrower margin of error, thanks to computer vision and convolution neural networks.
- *Robotic surgery*: Robotic surgery has a very small margin of error and can reliably execute surgeries 24 h a day without becoming fatigued. They are less intrusive than conventional techniques because of their high degree of precision, which can save the number of time patients need to recover in the hospital.
- *Vital stats monitoring*: Continual evaluation of a person's health is necessary to assess how well they are doing. Wearable technology is increasingly widely used; however, this data is not readily accessible and needs to be analyzed to provide useful insights. Numerous applications could save lives because vital signs can forecast changes in health even before the patient is aware of them [25] (Fig. 4).

AI of next-generation 3D printed medicines

Pharmaceutical 3D printing (3DP) pipeline and AI can work together. The administration of individualized medications must replace the long-standing "one size fits all" concept in medicine. Pharmaceutical 3DP can deliver customized medications in the clinic, but now it necessitates the presence and skill of qualified 3DP practitioners. There are numerous standard process optimization tools, including Finite element analysis (FEA), and mechanistic modelling, but none are capable of thoroughly optimizing the various stages of pharmaceutical 3DP [26]. In contrast, ML can offer intelligent optimization of each step in the creation of 3DP pharmaceuticals. This will eventually eliminate the requirement for ongoing expert input into the development of 3DP medicines, hence removing obstacles to the technology's clinical implementation [27] (Table 2).

AI with nanotechnology

Due to current molecular commodities longer production times, greater costs, and reduced productivity, AI has grown in significance in the pharmaceutical business, pharmaceutics, and medication delivery [28]. However, even the development of current formulations is based on time-consuming, pricey, and unpredictably error-filled research [29]. Big data, AI, and

Fig. 4 Advantages and disadvantages of AI

Table 2 Expectations and strategies of using AI in pharma industry

Company	Strategy of using AI
Expectation 1	Development of new drugs and biomakers
Novartis	In order to categorise digital images of cells treated with new chemicals and group the compounds with similar effects, Novartis is employing machine learning [27]
Berg	In more than 1000 cancer and healthy cell samples, an AI model was created to reveal previously undetected cancer pathways [27]
Wuxi NextCODE	Medicines that are developed and evaluated in clinical trials using powerful pattern recognition [27]
Expectations 2	Tackling of diseases which were difficult to treat earlier
Mission therapeutics	AI-assisted drug development for Deubiquitinase (DUB) inhibitors to combat Alzheimer's and Parkinson's [27]
Helax	Utilizes HealNet, an AI platform that helps scientists to identify more drugs for diseases while at the same time minimising pain, expense, and danger [27]
Expectations 3	Drug adherence among volunteers during clinical trials
CURATE	By optimising treatment dosage at the level of specific pattern, an AI-based platform was developed to halt the progression of advanced cancer disease [27]
Expectations 4	Better analysis and utilization of clinical data
BenevolentBio	Knowledge graphs are created using an AI platform that receives data from sources including academic papers, patents, clinical trials, and patient records [27]
Expectations 5	Finding the correct patients for clinical and reducing turnaround times
Santen and twoXAR	A platform for the discovery, screening, and prioritisation of novel medication candidates for ocular disorders was developed using AI [27]

multiscale modelling approaches are being integrated into pharmaceutics by a new system known as "computational pharmaceutics," which is proposing a significant potential change to the drug delivery paradigm. This system has emerged in response to the exponential growth of computing power and algorithms over the past decade [30]. In vivo pharmacokinetic parameters, drug distribution, physical stability, in vitro-in vitro

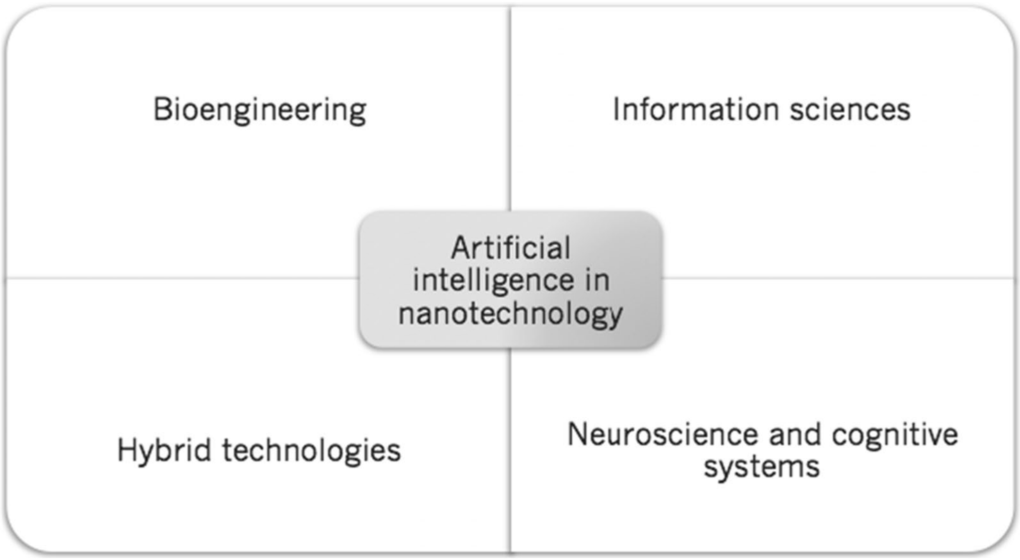

Fig. 5 AI in nanotechnology

correlation, and pre-formulation of physical and chemical properties and activity prediction are all examples of activities being done to apply AI techniques to pharmaceutical product development [31] (Fig. 5).

AI to predict new treatment

Improvements in AI, revived interest in treatments for rare diseases. Over 7000 uncommon diseases currently affect more than 350 million people worldwide. To research novel medications for uncommon disorders, Heal, a biotech company with headquarters in the (United Kingdom) UK, has acquired $10 million funding. Thera chon, another Swiss biotech firm, has been given $60 million to create medications for uncommon genetic illnesses [32].

Adoption of AI by the pharma industry

- Working with or acquiring tech companies and AI start-up many pharma companies make contact with specialised businesses and start-ups working on AI-powered drug discovery. This enables them to build promising therapeutic candidates based on known theories and experience using their knowledge and tools [33].
- Interaction amongst academics: As pharma starts to accept AI, partnerships between business and academics are anticipated to expand.
- Building internal expertise and supplying workers with the tools they need.
- Open scientific initiatives and R&D challenges: This useful AI adoption approach for drug research carries a lower financial risk than previous approaches [34] (Table 3).

Table 3 AI development

Aggregation and synthesizing information	Combines new ribonucleic acid (RNA) sequencing technologies with proprietary machine learning
Understanding disease mechanism	Analysis of genome-wide screens Provide detailed soatialn 3D structure of proteins Identity proteins involved in regulating the cell cycle Discovery of the next generation of therapies against cancer Training computer vision and medicine learning models
Generating novel drug candidates	Structure based deep (Convolutional neural network) CNN Screen compound libraries for efficacy against a disease Network-based machine learning approach Predict bioactivity of small molecules Identify biologic targets Predict the identity of each metabolite mass

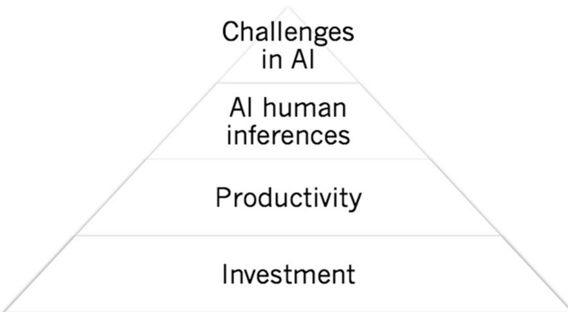

Fig. 6 Challenges in AI

Challenges that pharma company's face when attempting to adopt AI includes

- The technology's unfamiliarity, given its youth and esoteric nature, AI continues to be seen by many pharmaceutical businesses as a "black box."
- Inadequate IT infrastructure exists because the majority of IT programmes and systems in use today were not created or planned with artificial intelligence in mind. Even worse, pharma companies must shell out a sizable sum of money to improve their IT infrastructure.
- Since a large portion of the data is in free text format, pharmaceutical companies must take extra steps to gather and arrange it in an analytically-friendly manner. Despite these limitations, there is no doubt that AI is already changing the biotech and pharmaceutical industries [35] (Fig. 6).

Conclusion

AI has demonstrated its utility in a variety of drug discovery fields. AI can help scientists in the design, planning, quality management, maintenance, and quality control of pharmaceutical development and delivery. It is not a panacea and will not bring about seismic changes overnight, but it has the potential to increase efficiency, provide useful insights, and highlight novel perspectives in the pharmaceutical discovery process. Pharmaceutical companies are currently undergoing a revolutionary shift, with the risk being carefully managed in the development of novel science and practice. AI's success in the innovative drug research and development process will be measured by its integration of many unfamiliar and new areas. Data management, drug discovery, diabetes treatment, digital consulting, and other uses of AI are available in this field. There is substantial proof that medical AI can help doctors and patients deliver healthcare in the twenty-first century much more effectively.

Abbreviations

AI	Artificial Intelligence
DNN	Deep neural neutrons
ML	Machine learning
SVM	Support vector machine
NN	Neural network
DL	Deep learning
ANN	Artificial neural network
NLP	Natural language processing
QbD	Quality by design
3DP	3D printing
FEA	Finite element analysis
DUB	Deubiquitinase
CNN	Convolutional neural network

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Author contributions
AS: Drafting the article, Final approval of the version to be published. RM: Conception or design of the work. AR: Critical revision of the article. AM: Data collection, analysis and interpretation.

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