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Artificial Intelligence-Mounted Technologies Applied in Development of Pharmaceutical Products and Services: A bibliographic Review

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ABSTRACT

Researchers and practitioners are very interested in artificial intelligence (AI) as a way to make the kind of advance that the pharmaceutical business needs to make. Nevertheless, little research has been done on the function of AI and how it can change businesses. The report aims to pinpoint the precise ways in which artificial intelligence impacts the essential and auxiliary business operations of pharmaceutical firms. We present a qualitative study based on interviews with five big, five medium-sized, and five tiny pharmaceutical enterprises. We looked at which business processes within the pharmaceutical industry are susceptible to change and how, based on the scant literature on the topic. We find that tiny pharmaceutical enterprises have a major impact on the fields of master data management, human resource business, analysis and reporting, and research and development.

Background

AI grown into a subject that deals with issues in engineering, business, and medical. One application of AI is the development of expert systems. An expert system consists of an information base, a user interface, and an inference engine. AI has unique properties that allow it to reason and carry out activities that have the highest chance of achieving a given goal. AI does this by using a variety of algorithms that mimic even the most basic intellectual capacities of humans.AI is becoming more popular these days. Formulators have historically used statistical techniques for design space analysis, such as the response surface approach. Neural networks are used in the first method to simulate the way the human brain processes information. AI is becoming more popular these days. throughout many industries, with the pharmaceutical sector leading the way in this direction. Formulators have historically preferred statistical techniques, such as the response surface approach, The second way is the use of genetic algorithms, which use an evolutionary process to simulate the self-organizing and adaptable characteristics of biological systems. This study highlights the use of AI in the pharmaceutical production house for practical purposes, such as drug R&D, drug re purposing, improving pharmaceutical output, clinical testing, etc. These applications expedite the drug development process and lessen the requirement for human labor [2]. The pharmaceutical manufacturing company has made tremendous progress in digitizing References its data in the last few years. Because of this digitization, it is challenging to acquire, examine, and utilize this knowledge to address complex clinical problems. Because AI can handle massive volumes of data with more automation, it is utilized to address problem. It does not, however, pose a threat to human life on Earth. Hardware is used by AI.

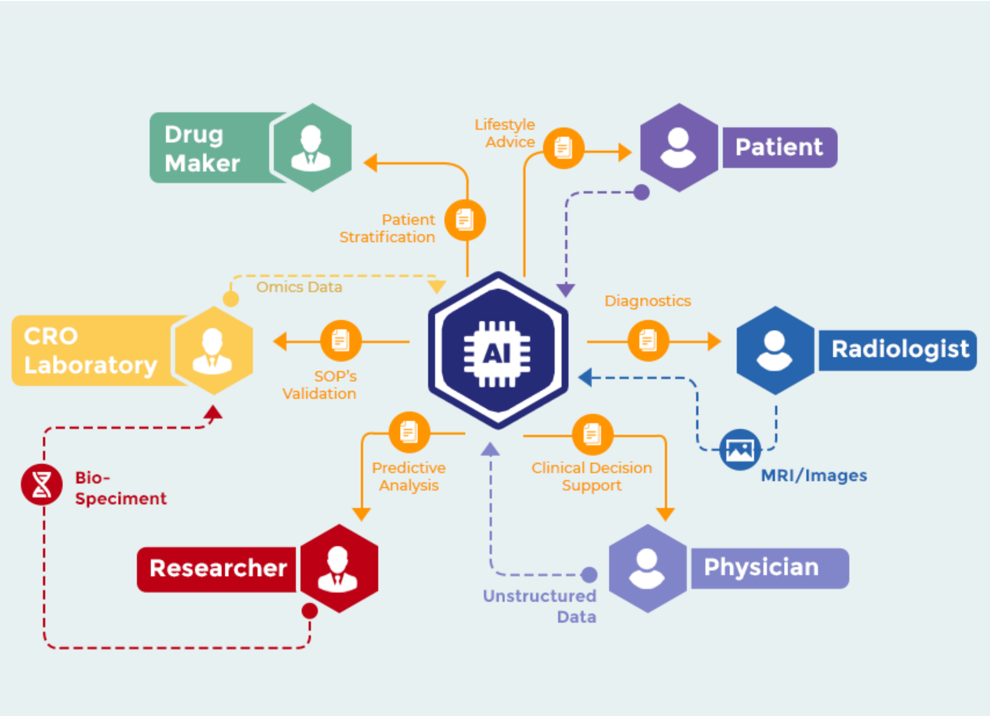

Fig. 1 Applications of AI in Pharma and Healthcare Industry

Tools, Technology, And Networks

Artificial neural networks (ANN)

The artificial neural network (ANN) is composed of multi-layer functional units that replicate the way electrical impulses are propagated in the human brain. These systems are primarily driven by biological factors. Neurons primarily function on the summation of all information and express an output; they take in input and learn directly from it [4].The neuron is the basic building block of biological neurological systems. Signals are received from one neuron and sent to other neurons via neurons, which are electrochemical cells [4]. Similar to people, the ANN system is made up of a main part called a "perceptron," or node. Artificial neurons are constructed in layers of nodes, analyzing input to produce an output that is delivered to the subsequent perceptron. Supervised learning (SL) and unsupervised learning are the two states that make up this category. Unsupervised learning involves the network taking in input data and using it to find patterns or structures that help to compress the data into a smaller format [5]. In Second Life, the network is "taught" by getting help while it learns. The network receives the pertinent input and output data in this SL. Through the network, a connection is made between the input and output data. According to several sources [4, 5], SL is the most often used and beneficial network for formulation. Network architecture refers to how linked neurons are arranged in a neural network.

Fuzzy logic

Fuzzy logic is another AI technology. Fuzzy logic is widely used by people to solve problems. It collaborates to comprehend the formulation and optimization process when ANN is present [4]. The concept of "true" or "false" is central to conventional sense. Therefore, this theory can be classified as either entirely incorrect or partially true. The membership function in the true set is 1 since the premise is true; in the false set, it is 0 [4].

Neuro-fuzzy logic

Giving in simple forms is fuzzy logic's central tenet.

To form it, neural network modeling is required. By definition, neuro-fuzzy logic consists of neural networks and fuzzy logic, as suggested by the name. It combines the generality and learning power of ANN with fuzzy logic's grasp of intricate ideas. Process data mining is ideally suited to neuro fuzzy logic. It is capable of expressing the linguistic IF_THEN rules and creating accurate models from data [4, 5].

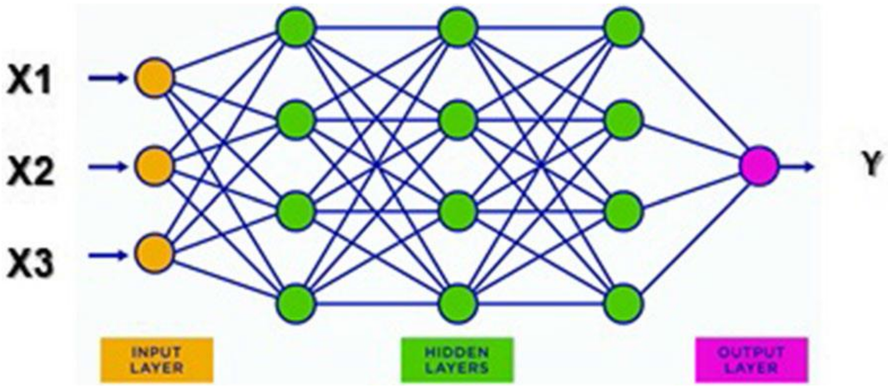

Fig. 2 Schematic diagram of artificial neural network

Genetic algorithm

To develop a pharmaceutical product, an optimization strategy is required to determine the optimal blend of substances and methods. It has been demonstrated by researchers that the ANN and GA combination offers the necessary tools for creating dosage formulations. GA is a biologically driven system, just like ANN. Its genetic variation's main concept, natural selection, mimics the essential ideas of evolution over generations. To determine which option is the best and most efficient, we use a genetic algorithm. They offer a "search" approach that works really well for optimization. The trial population would be advanced through an iterative process. We create a beginning population and assess each person's fitness as part of this process [4]. The "parents" of the ensuing generations are the fittest solutions. By adding some recombination and mutation, which creates a higher degree of new material in the pop, it becomes a more perfect response. An ANN and a genetic algorithm combine to create several possible solutions before the optimal one is determined. rhythmic are merged.

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Life cycle of pharmaceutical products

Artificial Intelligence has the potential to facilitate decision-making processes, facilitate logical drug design, identify the optimal treatment plan for each patient through customized medication, generate clinical data, and leverage that data to develop novel pharmaceuticals in the future [7]. It is logical to believe that artificial intelligence (AI) will play a role in the development of pharmaceutical goods, from the lab to the bedside. In order to foresee significant elements in pharmaceutical sales, Eularis developed the E-VIA analytical and decision-making AI platform. This platform uses machine learning algorithms and an intuitive UI to create analytical road-maps based on competitors, important stakeholders, and the market share currently held [8]. This increases stagnant sales and enables marketing executives to anticipate where to allocate resources. It also aids in their resource allocation for the best possible growth in market share.

AI in drug discovery

Artificial intelligence (AI) may be accepted by the pharmaceutical sector in part because of the time and money constraints involved in creating novel therapeutic compounds [11].By cutting down on the time and expense involved in finding new compounds, artificial intelligence (AI) tools and technologies can help the healthcare sector by quickly identifying hit and lead materials, validating drug targets, and optimizing drug structure design. AI still needs to overcome major data obstacles, such as the date's complexity, development, diversity, and ambiguity, despite these advantages [12, 13]. A range of in silicon techniques can be used to anticipate the chemical structure that would cause the intended reaction at the target site. Then, this structure can be enhanced to satisfy a number of requirements, including synthetic tractability, potency, safety, solubility, and permeability. The quantitative structure–activity relationship (QSAR) modeling tool has been used recently by researchers to filter out possible pharmacologic-ally active molecules from a million candidate pool. The enormous volume of data collected throughout the drug research and development process can also be handled by the deep learning approach, which is an advancement of the previous machine learning approach [15, 16].One can quickly anticipate huge amounts of chemicals or specific physio-chemical properties, such log P or log D, by using a computer model based on the QSAR. However, significant biological qualities like a compound's efficacy and undesirable side effects are just too complex for these models to predict with any degree of accuracy. Furthermore, there are problems with QUASAR-based models such as restricted exercise groups, inaccurate investigative data, and the requirement for additional trial validations. Researchers can use recently emerging AI techniques, such Deep Learning (DL) and relevant modeling principles, to solve these issues by using extensive data visualization and analysis to evaluate the efficacy and safety of pharmacological compounds [17, 18].
In 15 drug candidate-related absorption, distribution, and metabolism tests, DL models outperform conventional ML approaches.

AI in drug development

Numerous computational methodologies, including dissolving, porosity, instability concerns, and many more, can be resolved in the formulation design domain with the application of QSPR [23]. Depending on the photochemical characteristics of the medication, decision-support systems employ rule-based algorithms to select the type, nature, and quantity of recipients. In order to monitor and periodically adjust the entire process, they additionally employ a feedback loop [24]. In order to achieve the required dissolving profile, expert systems (ES) and artificial neural networks (ANN) were combined in a hybrid design process to create Paradoxical direct-filling hard gelatin capsules. The Model Expert System (MES) makes recommendations and judgments for formulation development based on the input parameters. Contrarily, ANN use back-propagation learning to establish a connection between the intended result and the formulation parameters, making the design of formulations easy. This is managed cooperatively by the control module [22]. Pharmaceutical product manufacturing could be greatly aided by the AI integration of these mathematical models. AI-infused technologies have developed into flexible instruments with a broad range of uses across the drug development life cycle. Identifying and verifying therapeutic targets, creating novel medications, re-purposing old ones, improving R&D effectiveness, compiling and analyzing biomedical data, and Drug combos, pharmacological traits, protein properties and efficacy, and drug re-purposing. The pharmaceutical business also utilizes AI to forecast possible synthesis methods for drug-like compounds [25], country, and drug-target interaction [34, 35].

Table 1 The AI techniques/tools used in the drug discovery process

Name of tools	Application
Reinforcement learning	used to maximize desired results and take into account a variety of interacting factors while optimizing drug combinations and dosages.
DeepChem	Deep learning resource for chemistry and drug discovery that is open-source
DeepTox	Open-source deep learning framework created especially for assessing and predicting toxicity
Neural graph fingerprints	An approach that uses neural networks to encode molecular structures as fixed-length feature vectors is appropriate for a number of drug discovery uses, including virtual screening, lead optimization, and property prediction.
PotentialNet	Prediction of ligand-binding affinity using a graph convolutional neural network (CNN)
Predictive ADME/Tox modelling	Tools that model and forecast the absorption, distribution, metabolism, excretion, and possible toxicity of medication candidates use machine learning approaches.
Natural language processing (NLP) tools	Help in gathering and evaluating data from patents, clinical trial data, and scientific publications
Cheminformatics tools	Chemical structures and properties can be analyzed and changed with the use of tools.
QSAR/QSPR modelling	Link biological activities or characteristics to molecular structures and attributes to predict compound behavior.
Deep learning (DL)	used in projects like de novo drug creation, virtual screening, and drug property prediction
Machine learning (ML)	assist in analyzing biological activity, predicting drug-target interactions, and improving lead compounds Fig. 3

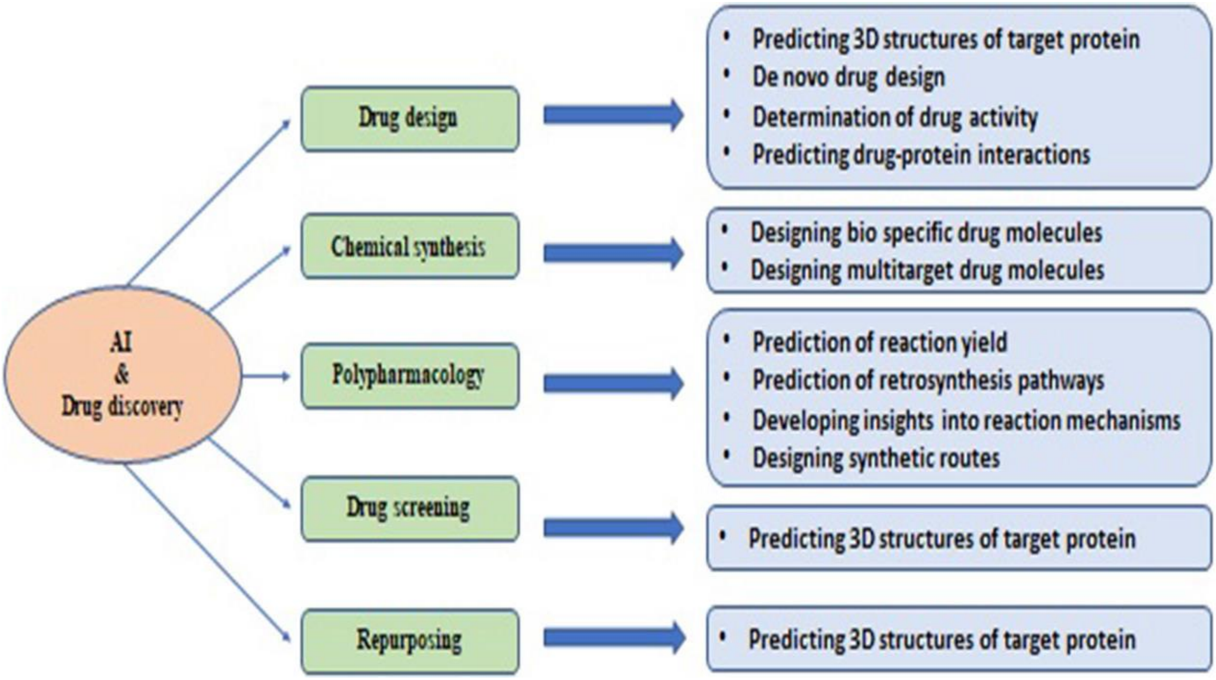

Fig. 3 Different applications of AI in drug discovery

AI in drug formulation

Various formulations, such as solid dispersion's, extrudes, pellets, nanoparticles, and liposome s, have emerged in pharmaceutical sciences alongside conventional dosage forms. The term "formulation techniques" refers to these methods since they facilitate the creation of formulations or add functionality to typical dosage forms like tablets. Because these techniques can effectively address a variety of API issues, such as low solubility, stability, bio-availability, and production capability, AI applications in formulation techniques are even more worthwhile to investigate in order to create next-generation drug products with desired efficacy and health outcomes [6].

Scaling up AI across the pharmaceutical value chain

AI and ML are causing revolutions in a number of manufacturing companies. However, industries pharmaceutical research, for example, is seeing a tremendous progress in these technologies. Artificial Intelligence is revolutionizing the distribution of life-saving drugs by re-structuring the value chain and gleaning insights from various data sets to ensure maximum interoperability. [24]

By enabling greater control with:, it could reduce operational costs and manual oversight in manufacturing operations.

• Quality assurance
• Using AI to automate robotic processes (RPA)
• AI prototypes to improve output and production
• Prognostic maintenance paired with AI to reduce appliance outages.

Pharmaceutical market of AI

AI is being used by pharmaceutical businesses to lower their financial expenses and failure risks. According to experts, the influence of AI will cause the pharmaceutical and medical industries to develop at a 40% annual pace between 2017 and 2024. Many pharmaceutical companies have made and are still making investments in AI. Additionally, they have collaborated with AI companies to provide vital healthcare solutions. One illustration is the collaboration on the treatment of serious kidney disease between the Royal Free London NHS Foundation Trust and Deep-mind Technologies, a Google company. Important pharmaceutical companies and AI firms are included in Figure 4.

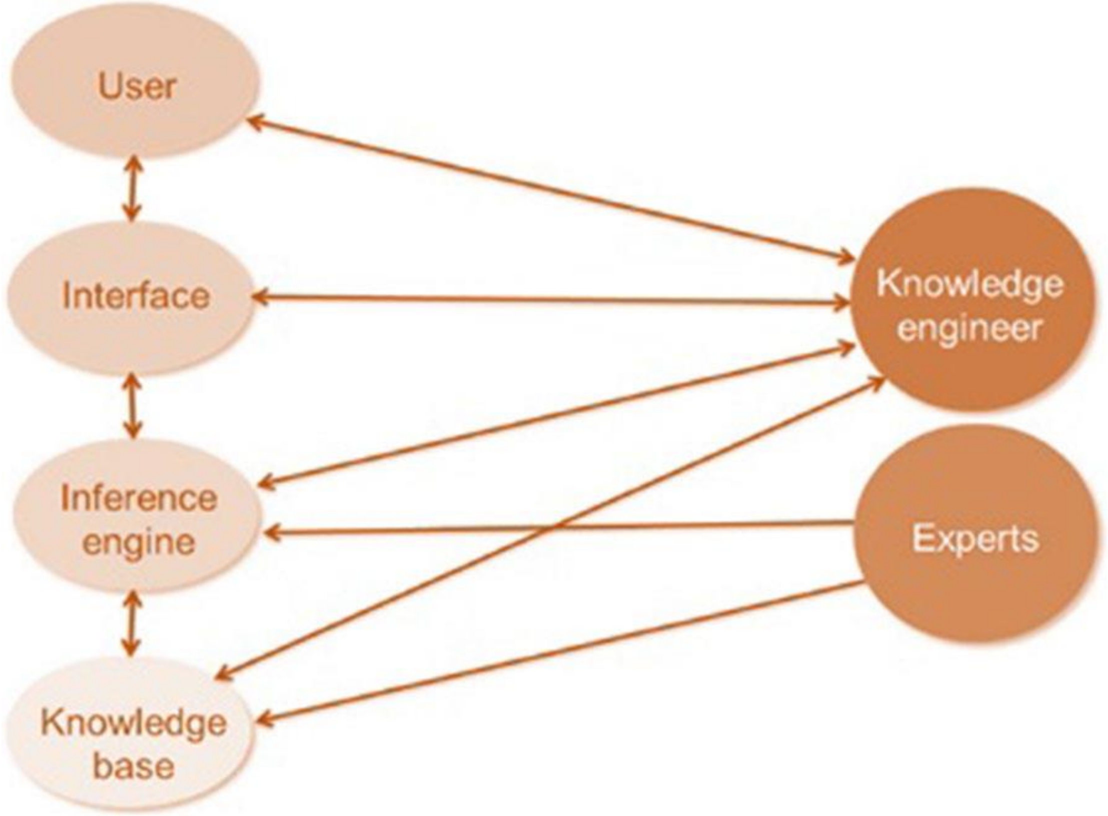

Fig. 4 Formulation of tablets and capsules uses rule-based systems

Predicting the mode-of-action of compounds using AI

Particularly excited are medicinal chemists about the potential of an AI platform that can forecast the on- and off-target effects of medications as well as their in vivo safety profiles before they are synthesized. The time, cost, and attrition rates required to develop novel drugs are decreased by the availability of such platforms. The toxicity of novel medications is predicted by Detox, and the likelihood of toxicity during clinical trials is evaluated by Proctor, two of these platforms [9, 10]. Through data sharing and exchange, the industry might potentially improve the predictive accuracy of these platforms if a precise and comprehensive datasets comprising information on the toxicity and therapeutic features of a wide range of medications becomes available.

Conclusion and future prospect

In summary, artificial intelligence is playing an increasingly important role in the formulation and development of pharmaceuticals, which is benefiting the sector in many ways. Artificial intelligence (AI) has already proven that it can analyze massive data sets, improve medication formulations, and expedite clinical trials. This has reduced the time and costs related to medication development while also increasing the accuracy and effectiveness of the entire process.

AI has promising futures in the formulation and development of pharmaceuticals. With AI's continued development and improvement, it is expected to play an even bigger role in drug development, helping scientists find new targets for drugs, interactions between drugs, and patient populations most likely to benefit from treatment. enabling scientists to create more individualized and efficient treatments.

Abbreviations

AI	Artificial intelligence
ML	Machine learning
R&D	Research and development
ANN	Artificial neural network
CNN	Convolutional neural network
SL	Supervised learning
DL	Deep learning
GA	Genetic algorithms
QSAR	Quantitative structural activity relationship
LDA	Linear discriminant analysis
NLP	Natural language processing
MES	Model expert systems
CFD	Computational fluids dynamics
DEM	Discreet element modelling
FEM	Finite element modelling
API	Active pharmaceutical ingredients
SD	Solid dispersions
SEDDS	Self-emulsifying drug delivery system
MLR	Multiple linear regression
PFES	Product formulation expert systems
RASAR	Read across structure activity relationship

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