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The application of Artificial Intelligence and Machine Learning to the Pharmaceutical Industry

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Abstract

The pharmaceutical industry is experiencing significant changes and is adopting new technologies at a faster rate than before. The application of 4.0 technologies increases the productivity and effectiveness of automated pharmacy processes, therefore, these technologies are driving the industry's growth. These include artificial intelligence (AI), machine learning (ML), internet of thing (IoT), big data, and other industry 4.0 technologies. This review will discuss the use of AI and ML in the pharmaceutical industry. Moreover, some pharmaceutical startups that implemented these technologies will be presented.

The pharmaceutical sector is going through major changes and rapidly embracing new technologies. The application of 4.0 technologies enhances the efficiency and productivity of automated pharmaceutical procedures, and as a result, these technologies are boosting the expansion of the sector. These technologies include big data, the internet of things (IoT), machine learning (ML), artificial intelligence (AI), and other 4.0 technologies.

The implementation of AI and ML in pharmaceutical science has gained an increased interest in the development and implementation of fast, efficient, and economical solutions. As a result, the number of startup companies that apply AI to this industry has grown rapidly in recent years. Table 1 shows various examples of AI-driven startups in the pharmaceutical field.

Table 1. AI-driven startups in the pharmaceutical field.

Startup name	Topic	Link
Atomwise	Application of AI to revolutionize small molecule drug discovery	http://atomwise.com
Exscientia	Combination of the latest AI technique with experimental innovation to engineer a new set of processes for drug discovery	https://www.exscientia.ai/
Cytel	Provision of statistical software and advanced analytics for clinical trial design and execution	https://www.cytel.com/
TrialSpark	Trial logistics simplification and the creation of a faster, more cost-effective clinical trial process	https://www.trialspark.com/
Glympse Bio	The improvement upon disease diagnosis, monitoring, and treatment with the use of non-invasive biosensor technology that measures protein activity	https://glympsebio.com/

AI has the ability to rapidly analyze and comprehend large amounts of data. Some applications of AI in the pharmaceutical sector include drug discovery and development, clinical trial design and analysis, personalized medicine, quality control and manufacturing, and supply chain management.[1]

Although there are various AI technologies in pharmaceutical sciences, such as natural language processing (NPL) or neural networks (NNs), ML is the most widely used branch of AI in this field. Furthermore, artificial neural network (ANN) is one of the most popular ML tool applied in drug design and discovery, particularly in quantitative structure-activity relationship (QSAR) studies; and in pharmaceutical pre-formulation and formulations.[2]

On the one hand, regarding drug discovery, ANNs have the potential to analyze large datasets of the properties of chemical structures to identify patterns and correlations. In addition, ANNs can predict the biological activity of new chemical compounds, which helps to design and develop new drugs, improving the effectiveness and efficiency of the process.

On the other hand, with respect to pharmaceutical pre-formulation, ANNs have the potential to predict the physical and chemical properties of pharmaceutical drugs, assisting in formulation optimization and performance enhancement. Furthermore, in the area of pharmaceutical formulation, ANNs have the potential to estimate the stability and bioavailability of new drugs.[3] They can also be employed to forecast how drug products would perform in diverse situations, such as different storage conditions, patient populations, and routes of administration.

In conclusion, the application of AI and ML, specially ANNs, has numerous benefits for the pharmaceutical industry. These benefits include improved efficiency, minimization of time and resources, enhanced accuracy, and cost savings.

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