

# Pharmaceutical Management in the Context Of Artificial Intelligence

Ana-Maria Pesterau<sup>1\*</sup>

Rodica Sirbu<sup>1</sup>

Emin Cadar<sup>2</sup>

<sup>1</sup>University of Medicine and Pharmacy, "Carol Davila", Bucharest, Romania

<sup>2</sup>"Ovidius" University of Constanta, Faculty of Pharmacy, Constanta, Romania

\*Email: rodica.sirbu3@gmail.com

## Abstract

The permanent trend of progress has led to new solutions applied to computer science and technology, these two elements have taken over all dimensions of science. Artificial intelligence (AI) is a branch of computer science that has penetrated all areas, from basic engineering to the pharmaceutical industry. Intelligence has found its way into pharmaceutical, medical, and healthcare applications. In recent times, conventional methods of drug design have been replaced by computer-aided drug design. Artificial intelligence is widely used to improve design techniques, the time needed for drug production, and to prevent drug interactions. Artificial intelligence technology and management in the pharmaceutical sector is used at every stage of the drug design procedure, which reduces health risks related to preclinical studies and also substantially reduces costs. Artificial intelligence-based pharmaceutical management is an effective tool for extracting fundamental pharmacological data, but it is also an advantage in the machine learning process.

**Keywords:** pharmaceutical management, artificial intelligence, technology, new drugs, medical management, healthcare system.

## Introduction

Good pharmaceutical management will certainly include the use of new methods of robotics and computer-assisted technology that will help the pharmaceutical market to be dynamic and come up with a solution to solve the pressing problems related, especially to the very numerous drug interactions detected in recent years in the medical and pharmaceutical fields.

Target proteins can be conveniently identified with the help of artificial intelligence, which increases the success rate of the designed drug [1].

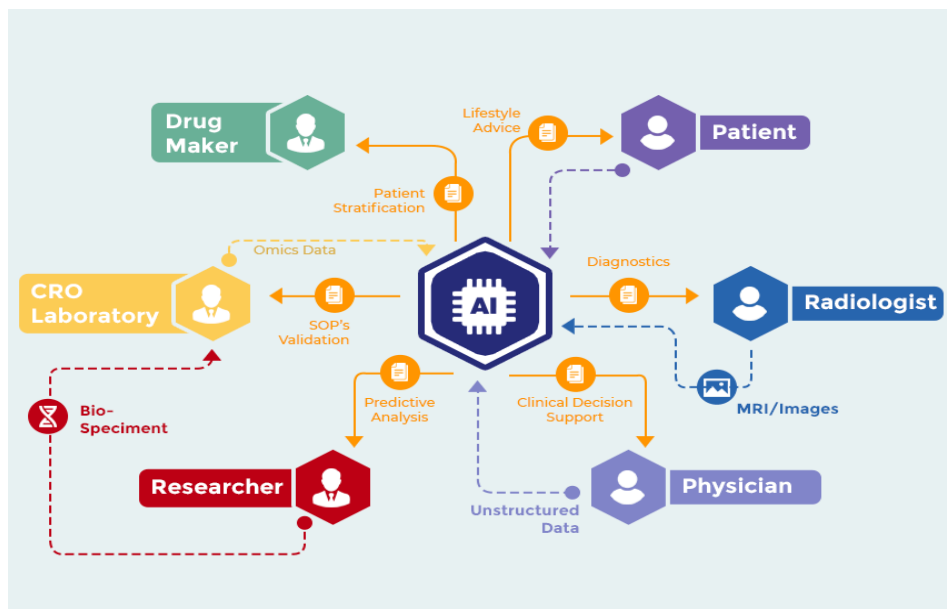
In this context of permanent technological development, artificial intelligence is intensively used in *de novo* drug design, activity evaluation, virtual screening, and *in silico* evaluation of the properties (absorption, distribution, metabolism, excretion, and toxicity) of a drug molecule [1].

A number of pharmaceutical companies have partnered with artificial intelligence companies for faster progress in drug development and in the healthcare system [2].

Technology plays a vital role in the development of science today, as well as in the medical sciences, including the development of the pharmaceutical process and lifestyle. This artificial intelligence will simplify work and increase not only productivity but also the quality of life and pharmaceuticals.

The main uses of AI management are in the following areas of interest:

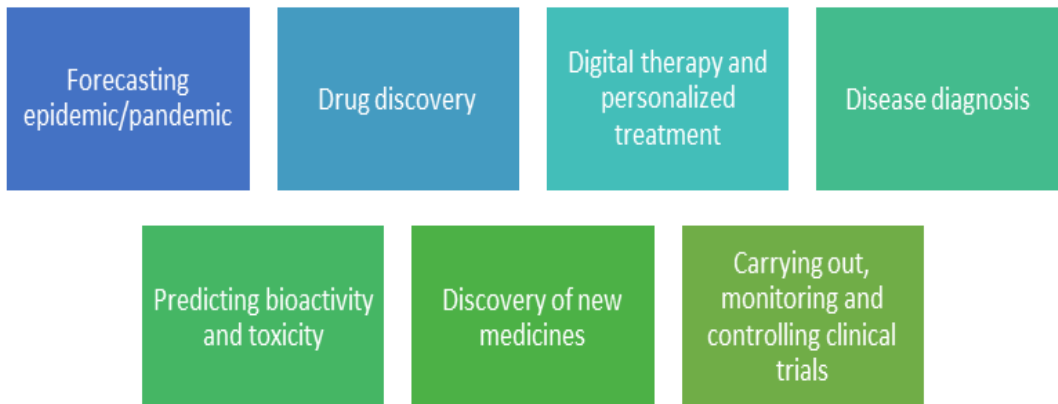
- Drug discovery;
- Diagnosis of certain diseases: digital therapy/personalized treatment: radiotherapy, cancer therapies, other chronic conditions;



**Figure 1 – Applications of artificial intelligence in pharma industry and healthcare**

- Drug-drug interactions;
- Prediction of bioactivity and toxicity;

- Clinical studies;
- Clinical trial design, patient identification, recruitment, and enrolment;
- Trial monitoring, patient adherence, and endpoint detection;
- Epidemic/pandemic prognosis.



## Figure 2 – Applications of artificial intelligence in medicine and the pharmaceutical industry

### Using artificial intelligence in new drug discovery

An example of artificial intelligence is Metastorm Marketing-Leading Software for pharmaceutical process lifecycle management and document management vendor frameworks. With Metastorm software, new products have been developed, and market strategies have been made easy to understand. It will bring together various strategies that will impart evaluation, efficient process execution, and accelerated value realization for organizations worldwide [3].

This software provides capabilities to design, automate, analyze, and monitor human-centric and integration-centric activities and processes, enabling pharmaceutical manufacturers to deliver new medicines in the most cost-effective and timely manner possible. It has a number of advantages such as repeatability, control, and gaining visibility across the organization while creating more efficient and streamlined processes [3].

The software helps pharmaceutical manufacturers quickly understand and leverage processes and systems to better manage their business, making it easier for pharmaceutical management to respond to ever-changing regulatory conditions and demands for a rapid product delivery lifecycle.

Advances in artificial intelligence could reduce the complexity and cost of drug discovery. Using a resource-based view, we conceptualize an innovation capability that measures a firm's ability to manage, develop, manage, and utilize artificial intelligence resources for innovation. Using patents and announcements of engagement to measure AI innovation capability can affect a firm's discovery of new drug-target pairs for preclinical studies [4]. The effect is pronounced for the development of new drugs whose mechanism of impact on a disease is known and for drugs at a medium level of chemical novelty. Artificial intelligence is less useful in drug development when there is no existing therapy, but also for drugs that are either completely new or "follow-on" drugs [4].

The drug discovery process requires navigating a combinatorial space of over 1060 molecules to find a suitable drug candidate [5]. This vast search space is simply too difficult to manage and process efficiently using technologies without artificial intelligence.

As a result, drug candidates for new discoveries by conventional methods are often clustered in small areas of the innovation space, and many of them offer only small improvements over existing drugs [7]. It is hard to find new drugs, especially those that differ substantially from existing drugs and offer large improvements [7, 8]. With new technologies, opportunities can be identified to accelerate the discovery of new compounds and the overall drug development process. Advances in artificial intelligence, especially with recent breakthroughs in digitization and machine learning, could help solve the problem of finding new drug structures [2]. Artificial intelligence accelerates the automation of predictions and the identification of hidden predictions in data, it facilitates recombination in innovation [9] accelerating the discovery of new chemical compounds under certain conditions.

### **Use Of Artificial Intelligence In Predicting Bioactivity And Toxicity**

Effectiveness depends on the affinity for the target protein or receptor. In similarity-based interaction, drug and target are considered and believed to interact with the same target [10]. Chem Mapper and the similarity ensemble approach predict drug-target interactions [11]. Substructure, connectivity, or a combination can also be considered [11]. Deep learning approaches have shown improved performance because deep learning is independent of 3D protein structure [11]. Deep prediction approaches to the interaction between affinity, protein, and drug molecules are approaches to circumvent toxic effects [12].

*In vitro* assays are common preliminary studies, followed by preclinical studies in which mortality can be distinguished and there is scope for further improvement. Several web-based technologies are accessible to reduce costs [13].

The Tox21 Data Challenge, organized by the National Institutes of Health, the Environmental Protection Agency, and the US Food and Drug Administration, evaluates computational techniques for estimating drug toxicity [14].

An algorithm called Deep Tox outperformed all procedures by recognizing static and dynamic features within chemical descriptors, while eToxPred was applied to estimate small molecule toxicity. TargeTox, a drug toxicity prediction based on biological targets, uses the guilt-by-association principle [14, 15].

A scoring function helps to predict the properties of novel molecules. ProCTOR could easily predict whether a drug will fail in clinical trials due to its toxicity. It also recognized adverse drug reactions [16].

Artificial intelligence is based on computation, geometry, and evaluation in collaboration with structure-based drug discovery by predicting protein structure [17]. Probability is necessary to understand its efficacy and effectiveness [18].

Different computational technologies can solve the problems encountered with quantitative structure-activity relationships [18]. Decision support tools use rule-based choice systems based on the nature and control of the amount of added ingredients to achieve a positive feedback process [19].

Given the increasing complications of better product efficiency and quality, manufacturing systems are attempting to give machines human knowledge [20]. Mixing technologies in the manufacturing process may prove to be a boost for the pharmaceutical industry.

## Conclusions

In the current context, researchers are interested in recent developments in artificial intelligence, especially its applications in healthcare, research, and pharmaceutical services. Smart hospitals and healthcare units equipped with artificial intelligence will change the shape of the future in the healthcare sector.

The management of the pharmaceutical industry is in continuous technological evolution, and artificial intelligence will be an opportunity to minimize the cost and time of drug development and treatment techniques, especially for chronic diseases. Research in recent years has focused on marine organisms in order to find new sources and alternatives to those already known that can be exploited to the maximum with low energy consumption, labor, and pollution. Proper pharmaceutical management will take into account robotics and incorporate artificial intelligence to avoid drug interactions and predict bioactivity, but also the toxicity of certain chemicals.

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