Letter to the editor

Contributions of Artificial Intelligence to Clinical Pharmacology

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Luz Olivia Bernal Regalado[1]*, Astrid Nicole Velásquez Castaneda[2], Marco Adriel Torres Castillo[3]

School of Medicine, Alberto Masferrer Salvadorean University, San Salvador, El Salvador.

* Correspondence
luzoliviab68@outlook.es

1. 0009-0004-5294-8896
2. 0009-0002-3420-2543
3. 0009-0003-9016-1579

Dear Editor.

It has been two years since the editorial "The world has changed" was published in volume five of this journal. It described how computer applications with Artificial Intelligence (AI) could contribute to healthcare. At that time, it was mentioned that the influence of AI in the different sectors of society would be of great significance despite of great relevance, despite the possible risks associated with its use.[i]

Indeed, we have seen that AI, a branch of computer science that runs computational platforms capable of simulating human intelligence, has evolved exponentially in recent years and promises to make significant contributions to the benefit of patients.[ii]

Through its disciplines, such as Machine Learning and Deep Learning, AI uses data and algorithms that process information and convert it into a language common to computer programs. This makes it possible to make predictions about certain items, solve problems, and make decisions.[iii,iv]

In particular, in the field of clinical pharmacology, AI has acquired a relevant and promising role in the development of new drugs. Through the analysis of large amounts of data, AI will be able to identify new pharmacological targets, macromolecules that recognize a drug and elicit a cellular response, as well as new biochemical pathways for obtaining different and innovative molecules.[iii,iv]

Thus, drug discovery and development based on machine learning algorithms that calculate more accurate data becomes an option to optimize traditional processes. This is particularly relevant, as it promises to reduce failure rates in drug development regularly and reduce the time spent in the process and the financial investment that is lost when only a few molecules make it past the clinical phase.[iii,iv]

AI is currently able to predict the processes of absorption, distribution, metabolism, and excretion of drugs, allowing for the optimization of drug synthesis and a reduction in the time required for drug development. The time and cost associated with the research and commercialization of a drug is approximately 16 years and several million dollars, respectively. However, the implementation of AI is estimated to reduce this time to less than three years.[iv,v]

To achieve these advances, there is an effort on the part of different entities, pharmaceutical companies, and the scientific community to exchange repositories of data generated from electronic medical records and results of scientific research on pharmaceuticals. These data allow, through machine learning models, to evaluate the pharmacokinetics and pharmacodynamics of a new drug, including those related to specific diseases such as Alzheimer's, Parkinson's, and Acquired Immune Deficiency Syndrome.[iv-vi]

Similarly, data obtained from electronic medical records also contribute to pharmacovigilance, i.e., the detection and evaluation of adverse drug reactions. Through tools linked to these registries, it is

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possible to extract data on adverse effects, drug resistance, and even clinical characteristics of patients that allow the study of drug-dose response. This is a confidential process, where the protection of personal data must be guaranteed.[iv]

In addition, the algorithms and statistical models obtained from machine learning offer the possibility of reusing drugs that were previously approved by the Food and Drug Administration (FDA) for the treatment of other diseases, with new medical indications, modifying the dose or even some molecule of the original form of the drug, making it more effective and efficient.[iii,vii] This strategy can also contribute to the discovery of therapies for rare and intractable diseases, reducing not only the cost and development time but also the risks associated with research into new drugs.[iv-vi]

Clinical trials have shown that the molecules have analogous chemical structures with similar properties, which bind to similar biological targets. Thus, common target genes between diseases allow repositioned drugs to share a mechanism of action.[iv] This promises to be an effective tool in the discovery and development of new molecules at lower cost and in less time, contributing to the implementation of successful pharmacological therapies with fewer adverse effects or for the management of diseases that have not responded to other drugs. Although there is still a long way to go, attention must remain focused on these new technologies that provide hope for patients.

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