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## Ethical Issues Arising from the Use of AI in Drug Discovery

*Georgia Livieri, Charikleia Anastasopoulou, Konstantina Briola, Panagiota Nikolopoulou, Iris Panagiota Efthymiou*

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## COMMENTARY

# Ethical Issues Arising from the Use of AI in Drug Discovery

## Georgia Livieri

PhDc in Bioethics and Health Policy, Cyprus International Institute for the Environmental and Public Health, Department of Health Sciences, Cyprus University of Technology; Research Associate, Cardiovascular Epidemiology and Genetics Research Lab, Cyprus University of Technology.

## Charikleia Anastasopoulou

MSc Linguistics; MSc Health Management, Speech Language Pathologist; ED Nurse, General University Hospital of Patras; Member of Hellenic Neuropsychological Society (HNPS).

## Konstantina Briola

PhD Candidate in Health Economics, Department of Economics, University of Piraeus; Research Associate, Laboratory of Health Economics and Management, University of Piraeus.

## Panagiota Nikolopoulou

BSc, Department of Electrical and Computer Engineering, Democritus University of Thrace.

## Iris-Panagiota Efthymiou

Adjunct Lecturer, University of Greenwich, UK; Researcher, Laboratory of Health Economics and Management, University of Piraeus, Greece.

## Abstract

Lately, the pharmaceutical industry has been implementing artificial intelligence (AI) in research in multiple ways for the purpose of drug discovery. AI has great benefits to offer by performing tasks that a human may not be capable of. However, it also raises many ethical issues that need to be resolved. After describing the general picture, this paper explores the benefits and disadvantages of AI and attempts to find answers to the challenges it poses in order to make sure that its use will be ethical, fair, unbiased and beneficial to people. The challenges addressed below focus on ensuring patients' safety from biased AI algorithms and violation of their data privacy, the need to train and inform staff properly, as well as the necessity of achieving an optimal level of trust towards AI. In the end, some policy recommendations are being presented, aiming to contribute to the centralized approach and to the balanced sense among the uses of AI. The key to success is always taking into account human agency in order to make AI's use transparent and robust, while minimizing its risks.

**Keywords:** Artificial Intelligence, Drug Discovery, Algorithm Bias, Data Security, AI Ethics

## Introduction

Lately, the use of artificial intelligence (AI) has been increasing in various scientific sectors and is being implemented in research with multiple ways. The pharmaceutical industry is no exception, as it

currently utilizes different applications of AI for a large variety of purposes. This shift of focus on AI is justified by the recent, drastic increase of data digitalization that has occurred the past few years, as AI algorithms are known to be more efficient when using large amounts of data as input.

Although a global definition of AI does not exist, it is typically used as a general term to describe the stimulation of human intelligence by machines, being programmed to think like humans and mimic their actions. Thus, AI machines are capable of analyzing and processing data, extracting conclusions from it, making decisions, receiving inputs from their environment and learning from such input (Lamberti et al., 2019).

In the pharmaceutical industry AI has proven to be a useful tool for discovering new, efficient drugs. AI applications are currently used for drug identification and validation of drug targets, design of new drugs, improvement of research and development (R&D) efficiency (Mak & Pichika, 2019), decision making, determination of suitable treatments for a patient, including personalized medicine, and management of the vast amount of clinical data (Paul et al., 2020).

It becomes apparent that AI can assist the future of drug design in the pharmaceutical industry. However, promising as it sounds, it does not come without challenges, as there is still a lot of skepticism, when AI is involved. The use of AI in the pharma industry raises many ethical issues, therefore in order for science to implement AI efficiently; those ethical issues must be resolved.

## **Artificial Intelligence in the Pharmaceutical Sector**

Artificial Intelligence (AI) is being deployed by companies at a phenomenal speed, however as AI becomes mainstream, many people have raised serious concerns about the ethical implications arising from drug discovery and development process. Below the most crucial ethical challenges are being discussed.

### ***Algorithm bias may harm some social groups***

Artificial Intelligence uses algorithms to evaluate data from the world, to present and to draw conclusions. However, it can suffer from bias having an adverse effect on social groups, especially in the field of health, making wrong decisions (Panch et al., 2019).

Inequalities that support bias already exist in society and are affected by parameters, the creator and their purpose. In every algorithmic bias lies an issue of society that combines all existing inequalities, socioeconomic status, race, ethnic origin, religion, gender, disability or sexual orientation, and many more. Each time the algorithm is applied the qualitative and quantitative characteristics of the groups may differ (Panch et al., 2019). However, treating algorithmic bias as a simple technical issue, we have

only engineering solutions, but without solving the real problem, the inequalities of data and values (Sánchez-Monedero et al., 2020). As long as our perspective on our questions is limited, then this will be reflected in data, either directly or consequently in the final decisions and results.

Dealing with algorithmic bias means reducing it, since data and value inequalities exist in our society, and even the current legislation is unable to eliminate them. The more general use of an algorithm, the greater the risk of harming social groups due to its sensitivity and specialization (Sánchez-Monedero et al., 2020, Mehrabi et al., 2019). Interdisciplinary teams of researchers are the ones who can refine the algorithm development process in order to optimize performance and at the same time minimize bias and arrive at fairer AI decisions.

### *Data Security*

Due to the complexity of medical data and the need to share large volumes of data in the pharmaceutical and technology sectors, data security concerns are growing. There can be many risks when using and transferring such data. The ways in which data privacy can be violated are, among others, indirect data leakage, data poisoning, linkage attacks, dataset reconstruction from published results, adversarial examples, transferability attacks, model theft, etc. (Niranjana & Chatterjee, 2021).

Despite the risks, many patients consent to the collection and use of their personal data in order the healthcare and research to be improved (Elysse et al., 2020). Although this move seems sufficient to protect their personal data, other problems and questions arise through this agreement. It is a common phenomenon for the patient to sign up to extensive terms and conditions before each episode of care or agree to future uses of their data that they have not been informed of yet (Elysse et al., 2020).

Data privacy is a central issue in training and testing AI models, including many different strategies developed to achieve data security. Finally, testing AI models in real-time clinical situations in order to further understand the fragility of such models and where their vulnerabilities can be exploited, can be devised to counter the problem (Niranjana & Chatterjee, 2021).

### *Staff Training and AI*

As we move into the era of digitalization, keeping employees up-to-speed constitutes a huge challenge for the sector itself. In order for pharmaceutical companies to gain competitive advantage, they need well-trained employees around AI at all levels of the hierarchy (Aydogdu, 2012). In addition, due to the rapid changes in the procedures and regulations to be followed by pharmaceutical companies, the training process should be in short periods of time (Aydogdu, 2012).

As artificial intelligence evolves in healthcare, there is a chance to be an increase in demand for new skill sets, such as computer science (Indrajit, 2020). Therefore, when referring to a group of people who will develop artificial intelligence and machine learning technologies to improve clinical trials, personalized medicine and drug discovery, everyone in the group should automatically have basic biological and chemical knowledge, let alone programming skills.

### ***Reliability of AI predictions***

Technological advances in the capabilities of AI will contribute to the transition from the automation of repetitive and well-defined tasks to guiding decision-making under uncertainty which is undertaken only by medical professionals so far (Asan et al., 2020). By the time that healthcare providers rely more and more on AI, the so-called calibrated trust (Hoffman et al., 2013), meaning the proper trust relationship, constitutes a requirement for effective decisions.

The reliability of an AI technology is built on the user itself and his/her input data. Cultivation of trust in AI can be influenced by many human factors such as user educational level, previous experiences, user biases and perception towards automation, as well as properties of the AI system, including controllability, transparency and complexity of the model, associated risks and many more (Asan et al., 2020). Additionally, to the above mentioned, taking into consideration that an AI system might be trained with insufficient and subjective data from different sources, AI could generate biased or overfitted outcomes which might not be aware of the clinical user (Asan et al., 2020).

Profoundly, these concerns prevent users from trust and accept AI systems. The development of AI must be built on mechanisms that will establish a properly balanced, high-level trust from and to the user that matches the capability of the AI system (Lee & See, 2004). Fairness, transparency and robustness should be taken into serious consideration when developing AI in order to reach the highest level of trust.

### ***Fear of AI replacing the staff in drug industry***

Definitely, despite the fact that AI saves lives and assists businesses in thriving, there is still a main fear that it will destroy livelihoods (Mohanty, 2019). Doubtlessly, jobs traditionally used to be done only by humans have now been replaced by AI. On the other hand, it is of crucial significance to note that AI creates new job opportunities, since it needs people to undertake the training and monitoring process. At its best, AI works in collaboration with people instead of in placing them, putting emphasis on removing the tedious parts of jobs so employees can focus on constructive things, undertaking tasks that humans were unable to, and helping employees improve their jobs (Mohanty, 2019).

In the drug industry, artificial intelligence can take on tasks that human minds simply cannot do. According to a study from Tufts University, the process of developing a drug from the beginning to approval to market is time consuming and up to an extravagant cost. Due to the fact that most drugs fail to reach market close to the final stage, hence lots of money has been spent; AI may contribute in lowering the rate of failed trials through leveraging the vast amounts of data regarding medicine and health (Mohanty, 2019). Additionally, it may assist in finding the proper patients-participants in clinical trials, modelling the behavior of molecules to improve prediction on how they will behave in the human body and searching for genetic biomarkers that allow medicine to be tailored to individuals (Mohanty, 2019).

## **Conclusions & Policy Recommendations**

At this point a revolution to the overall drug development process is being required, since the expenditure on drug development increases exponentially (Kim et al., 2020). Doubtlessly, AI in the field of drug development has been at the center of attention lately, so it is of high priority to demonstrate that in order to make drug discovery more successful it is impossible to achieve better decisions with the current ways of generating and utilizing data (Bender & Cortés-Ciriano, 2021). Definitely, we cannot overlook the apparent benefit in several areas of human daily life that artificial intelligence can offer. As Efthimiou has mentioned, using technological achievements, meaning AI, Big Data, e-health, m-health apps, can be the direction leading to the amelioration of the quality of the provided services and to dealing with the new challenges that will be about to arise in the health sector (Efthymiou et. al. 2019). In this path, countries should implement a centralized approach and make policies that balance the need to develop artificial intelligence with the desire to have protection around its use (Timan & Mann, 2019).

To deeply improve the field, it is necessary to penetrate into biological advancements and generate data containing a signal of interest guiding by a hypothesis-driven manner, related both to efficacy and safety endpoints (Bender & Cortés-Ciriano, 2021). That practically means that we need to support clinics with well-trained candidates, validate targets with better methods, improve patients' recruitment process and make advances on the way clinical trials are conducted. Last but not least, the ethical validity of AI algorithms should be assessed; either based on standards or protocols (Jobin et al., 2019) or by ethics consultants that will cooperate with engineers in the stage of development. "Trust-worthy" is a prerequisite when planning AI, while human agency and oversight should be taken into account, as well. What is more, other factors that play crucial role are technical robustness and safety, privacy and data governance, transparency, diversity, non-discrimination and fairness, societal

and environmental wellbeing and accountability (Krzysztof, 2020). Human-centered solutions embedded in AI procedures and algorithmic impact assessments obviously remain the goal for minimizing the risk of discrimination, while using AI/ADM tools (Joyce et al 2021).

All in all, we are facing an era in which AI is going to be developed, and that is why we should make sure beforehand that this will happen in the right track, serving people's best interests. Only then will AI be capable of making drug discovery and design easier, quicker and more efficient.

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