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To explore the pharmacological mechanism of action using digital twin

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ABSTRACT

With the advent of medical technology and science, the number of animals used in research has increased. For decades, the use of animals in research and product testing has been a point of conflict. Experts and pharmaceutical manufacturers are harming animals worldwide during laboratory research. Animals have also played a significant role in the advancement of science; animal testing has enabled the discovery of various novel drugs. The misery, suffering, and deaths of animals are not worth the potential human benefits. As a result, animals must not be exploited in research to assess the drug mechanism of action (MOA). Apart from the ethical concern, animal testing has a few more downsides, including the requirement for skilled labor, lengthy processes, and cost. Because it is critical to investigate adverse effects and toxicities in the development of potentially viable drugs. Assessment of each target will consume the range of resources as well as disturb living nature. As the digital twin works in an autonomous virtual world without influencing the physical structure and biological system. Our proposed framework suggests that the digital twin is a great reliable model of the physical system that will be beneficial in assessing the possible MOA prior to time without harming animals. The study describes the creation of a digital twin to combine the information and knowledge obtained by studying the different drug targets and diseases. Mechanism of Action using Digital twin (MOA-DT) will enable the experts to use an innovative approach without physical testing to save animals, time, and resources. DT reflects and simulates the actual drug and its relationships with its target, however presenting a more accurate depiction of the drug, which leads to maximize efficacy and decrease the toxicity of a drug. In conclusion, it has been shown that drug discovery and development can be safe, effective, and economical in no time through the combination of the digital and physical models of a pharmaceutical as compared to experimental animals.

1. Introduction

Using animals for science is widespread all over the world. Rats, mice, hamsters, rabbits, fish, birds, guinea pigs, amphibians primates, dogs, cats, and other animals have long been used in pharmacological science (NRC, 2010). An estimate of 192.1 million animals was used for research purposes in 2015 globally (Taylor and Alvarez, 2019). With the advancement of research and development in medical technology, the number of animals used in research has increased. For a long time, the suffering, misery, and death that animals suffer during laboratory experiments have been a point of contention (Doke and Dhawale, 2015; Festing and Wilkinson, 2007). Therefore, evaluation to identify potentially successful drugs prior to model validation is necessary. The biggest challenge of 21st-century pharmacology, to explain the pathways of a drug to push new methods and creativity. To prescribe the appropriate drug to the right individual it is important to understand their

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