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This article talks about the difficulties in finding medicines. It explains that many medicines fail in clinical trials, which is expensive and time-consuming. To solve this, laboratory methods and computer models are used, but they are not perfect for predicting the effects of medicines on humans.

Then, it talks about AI, which helps to better assess medicines. It's like computers learning from existing data. But current models still have gaps in predicting certain effects of medicines.

It talks about "big data," which means a lot of data. This poses challenges because this data needs to be analyzed quickly and accurately. Better techniques will need to be developed to use all this information in medicine research.

We discuss the major impact of big data on medicine discovery. Big data represents large volumes of complex information that require specialized tools to be analyzed. Initiatives such as PubChem and ChEMBL serve as huge repositories containing data on chemicals and their biological interactions. These databases are constantly updated with new information, providing a crucial resource for researchers in the field of medicine discovery.

In summary, the advent of big data has transformed the landscape of pharmaceutical research, opened new possibilities while also posing new challenges to overcome.

Big Data in drug discovery has become crucial with the growth of databases, notably PubChem, ChEMBL, and DrugBank, providing information on millions of compounds and biological targets. The use of this massive data requires innovative computational approaches, including deep learning, to predict drug effectiveness and side effects. However, these data present challenges, including missing data and biases in biological responses, which must be overcome to obtain accurate models. The evolution of artificial intelligence, transitioning from machine learning to deep neural networks, has enabled significant advancements in this field, harnessing the power of data and new hardware. Initially, for studying drugs, simple information about their chemical structure was used. But over time, new ways of looking at these drugs were developed, using more advanced computer tools. These tools help us to see more complex details and better predict how drugs may work. We also started using machines to learn from large amounts of data about drugs. This allowed us to create more accurate models for predicting how drugs will act in the human body. All of this was made possible by improvements in computers and the increase in information we have about drugs.

Researchers held competitions to see which approach was best for discovering new drugs. In one of these competitions, called DeepTox, a computer model based on deep neural networks outperformed other models based on classic machine learning approaches. Since then, many studies have been conducted to use deep neural networks in drug discovery. For example, one study developed a model based on these networks to predict how drugs interact with their biological targets. This study used a database called DrugBank, which contains information on thousands of drug-target pairs. Deep neural network-based models have also been used to predict several biological effects of drugs simultaneously, yielding better results than traditional models. Despite these successes, there have been conflicting reports on the effectiveness of deep neural networks compared to traditional machine learning methods, and as deep neural networks are relatively new in this field, there are no universal criteria yet for choosing the right modeling parameters or building the right modeling process.

To create computer models that help to discover new drugs, we relied on fairly simple chemical features. But then, new ways of describing molecules were developed, allowing for more precise and comprehensive models. We also used more advanced learning methods to create these models, making them more sophisticated and able to handle more complex data. Then, to make sure these models worked well, we started testing them more thoroughly. All of this has greatly contributed to improving our understanding of how drugs act in the body.

Personalized medicine aims to tailor treatments based on the individual characteristics of each patient, such as their genetic and molecular profile. This allows for better prediction of how each person will respond to a specific treatment. Through studies on biomarkers, many genes involved in human diseases have been identified, leading to a better understanding of individual responses to treatments. This approach also relies on the use of computer models to analyze genetic data and identify patterns of genetic variability in the population. For example, the NIH's Precision Medicine Initiative supports the creation of databases to share genomic data and facilitate personalized medicine. While genome sequencing analysis is not the focus of this article, it plays a crucial role in personalized medicine and benefits from artificial intelligence techniques.

In conclusion, AI offers promising opportunities to accelerate drug discovery by reducing costs and time. Recent advances in deep learning modeling show advantages over traditional approaches and are increasingly being used in all areas of drug discovery. AI offers promising prospects for accelerating drug discovery and personalizing them for each patient. By using advanced computer methods, such as deep learning, researchers can analyze large amounts of data to predict the effectiveness of drugs and their potential side effects. This saves time and resources by identifying the most promising drug candidates more quickly while reducing risks for patients. The successful application of AI in this field requires close collaboration between scientists and healthcare professionals to ensure accuracy and reliability of the results. Despite persistent challenges related to data availability and quality, as well as drug safety, AI offers considerable potential to revolutionize drug discovery and development, paving the way for better health and more effective treatments for patients worldwide.