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Machine Learning Applications in Drug Discovery

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Editorial

The use of machine learning in drug discovery is expanding, aiding research in a variety of areas. The increasing number of pharmaceutical businesses that use ML as part of their business model demonstrates ML's success. The goal is to lower the resource and labour requirements of drug development, specifically the high throughput screening (HTS) technique. Another goal of ML is to eliminate the necessity for animal testing, which has recently attracted unwanted attention.

ML algorithms and software have been developed and used at all stages of drug discovery and development, including clinical trials, to identify novel targets, provide stronger evidence for target– disease associations, improve small-molecule compound design and optimization, increase understanding of disease mechanisms, increase understanding of disease and non-disease phenotypes, develop new biomarkers for prognosis, progression, and drug efficacy, and improve a variety of outcomes. Traditional MLTs have been intensively investigated in drug discovery. k-Nearest Neighbour (kNN), decision tree, random forest, support vector machines (SVM), artificial neural networks (ANN), principal component analysis (PCA), and k-means are examples of supervised and unsupervised MLTs. Their attractiveness arises from their simplicity, which is computationally undemanding yet providing better prediction accuracy than typical predictive algorithms. Non-computer scientist researchers can also understand the underlying processes of traditional methodologies [1].

Innovative drug discovery approaches

AI can identify hit and lead compounds, as well as providing faster validation of the drug target and optimization of drug structure design. A computational model based on the quantitative structure-activity relationship (QSAR) can swiftly predict a large number of chemicals or simple physicochemical parameters. Based on big data modelling and analysis, DL and relevant modelling studies can be used to evaluate the safety and efficacy of medicinal compounds. Numerous in silico methods for virtual screening compounds from virtual chemical spaces, as well as structure and ligand-based methodologies, allow better profile analysis, faster elimination of non-lead compounds, and therapeutic molecule selection at a lower cost. To pick a lead ingredient, drug design techniques such as coulomb matrices and molecular fingerprint recognition examine the physical, chemical, and toxicological characteristics [2,3].

Reinforcement learning: RL differs from supervised and unsupervised learning in that it is a type of continuous learning that is autonomous. This is due to the fact that RL algorithms make decisions, whereas most supervised and unsupervised algorithms create predictions. Because of RL's capacity to respond quickly to dynamic settings, it is employed in gaming, robotics, and financial trading. Indeed, there are situations where RL outperforms supervised learning on classification problems, but the ability of RL to train continuously with minimal human intervention is required.

Transfer learning: If data is few, there are strategies that can be employed to get around this challenge. Transfer learning is one such strategy, which is the process of transferring knowledge gained from one work to another. Transfer learning is a prominent ML framework that incorporates a variety of approaches, particularly in medical picture categorization.

Multitask learning: The advantages of multitask learning are especially effective in low-volume data sets and/or when noise is present. Furthermore, multitask learning was found to outperform classical MLT, especially when data was scarce. Using a neural network as an example, a typical design learns a single task at a time and produces a single layer for the prediction job [4,5].

Drug development applications

Target identification and validation: The gold standard in drug development is to create medications (small molecules, peptides, antibodies, or newer modalities such as short RNAs or cell treatments) that affect disease status by regulating the activity of a biological target. Despite a recent comeback in phenotypic screens, starting a drug development programme necessitates the identification of a target with a valid therapeutic hypothesis: that changing the target will change the disease state. Target identification and prioritising refers to the process of selecting a target based on the evidence provided.

Small-molecule design and optimization: Much effort has been done to adapt DL approaches to ligand-based virtual screening, such as multi-task neural networks. Compounds with comparable chemical structures can be identified computationally given a lead substance. Traditionally, this has been done with traditional statistical approaches, however multi-task DNNs are proving to be more effective. When inferring the properties and actions of tiny compounds, DNNs can greatly improve prediction power. The one-shot learning technique can greatly minimise the quantity of data needed to make valid predictions about a molecule's readout in a new experimental setup [1,2].

Predictive biomarkers: ML-based biomarker identification and drug sensitivity predictive models have been shown to aid in improving clinical success rates, better understanding a drug's mechanism of action, and identifying the correct drug for the right patients. Building, validating, and applying predictive models earlier, using preclinical and/or early-stage clinical trial data, will be most beneficial. Late-stage clinical trials take many years and millions of dollars to conduct, so it will be most beneficial to build, validate, and apply predictive models earlier.

AI in drug screening

Physicochemical features of a drug, such as solubility, partition coefficient (logP), degree of ionisation, and intrinsic permeability, have an indirect impact on its pharmacokinetic qualities and target receptor family, and must be taken into account while developing a new medicine. Physicochemical qualities can be predicted using a variety of AI-based methods. To train the computer, ML, for example, employs massive data sets generated during compound optimization. Molecular descriptors, such as SMILES strings, potential energy measurements, electron density around the molecule, and atom coordinates in 3D, are used in drug design algorithms to produce viable compounds via DNN and forecast their attributes.

The affinity of drug molecules for the target protein or receptor determines their efficacy. Drug molecules that do not interact with or have a high affinity for the targeted protein will not be able to provide a therapeutic response. It's

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also possible that produced therapeutic compounds interact with unwanted proteins or receptors, resulting in toxicity in rare cases. As a result, DTBA (drug target binding affinity) is critical for predicting drug–target interactions. AI-based approaches can assess a drug's binding affinity by looking at the traits or similarities between the drug and its target. To determine the feature vectors, feature-based interactions recognise the chemical moieties of the medication and the target [2].

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Conflict of Interest

The author reported no potential conflict of interest.

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