عنوان مقاله:

An overview of artificial intelligence-based drug toxicity prediction tools

محل انتشار:

اولین کنگره بین المللی هوش مصنوعی در علوم پزشکی (سال: 1402)

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خلاصه مقاله:

Background and aims: In the drug manufacturing field, unexpected toxicities are a major causeof attrition during clinical trials and post-marketing safety concerns cause unnecessary morbidityand mortality. However, animal model-based toxicity predictions have been demonstrated toagree only ۴۳% and ۶۳% of the time in rodents and non-rodents, respectively, when extrapolatedto humans, and less than ۳۰% when it comes to predicting adverse drug reactions (ADRs) in thetarget organs. Therefore, the elimination of potential new drugs based on toxicological safetystudies, conventionally based on animal models, is controversial. Pharmacovigilance (the sciencethat monitors, detects and prevents ADRs) is increasing its efforts to develop in silico models,taking advantage of the large amount of recently available data that present a great opportunityfor the use of techniques based on artificial intelligence, neural networks and deep learning currentmodels. The most representative and recent examples of the application of AI techniques todetermine the toxicological properties of new drugs are discussed in this article.Method: This study is a review of published articles since ۲۰۱۲ in the field of artificial intelligenceand toxicity in drug discovery. In order to collect the articles, the keywords of “Drugdiscovery”, “Toxicity”, “Artificial intelligence”, “Deep learning” and “Machine learning” wereused in databases such as Google Scholar, Science Direct, PubMed and etc. The criterion for theapproval and review of the articles was the use or introduction of the latest methods based on artificialintelligence, machine learning and deep learning in the field of drug toxicity detection. Also,open source databases with molecular or pharmaceutical information like DrugBank, ChEMBL,PubChem and SIDER have been used for more detailed investigations.Results: The classification of the best and most representative methods based on artificial intelligence,neural networks, machine learning and deep learning has been performed in the predictionof specific toxicities such as drug-induced liver injury, skin sensitization, cardiotoxicity, chemicalcarcinogenesis, cytotoxic effect, seizures, hemolytic toxicity, plasma protein binding, phototoxicityand neurotoxicity. The presented methods and models for predicting drug toxicity in eachorgan were compared in terms of specificity, accuracy, and sensitivity. The models and methodsexamined in this study include a variety of models such as Bayesian, Support Vector Machine(SVM), Bernoulli Naive Bayes, AdaBoost decision trees, Random Forest (RF), ...

کلمات کلیدی:

artificial intelligence, drug discovery, toxicity, deep learning, machine learning