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A renaissance of neural networks in drug discovery

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Abstract

© 2016 Informa UK Limited, trading as Taylor & Francis Group.Introduction: Neural networks are becoming a very popular method for solving machine learning and artificial intelligence problems. The variety of neural network types and their application to drug discovery requires expert knowledge to choose the most appropriate approach. Areas covered: In this review, the authors discuss traditional and newly emerging neural network approaches to drug discovery. Their focus is on backpropagation neural networks and their variants, self-organizing maps and associated methods, and a relatively new technique, deep learning. The most important technical issues are discussed including overfitting and its prevention through regularization, ensemble and multitask modeling, model interpretation, and estimation of applicability domain. Different aspects of using neural networks in drug discovery are considered: building structure-activity models with respect to various targets; predicting drug selectivity, toxicity profiles, ADMET and physicochemical properties; characteristics of drug-delivery systems and virtual screening. Expert opinion: Neural networks continue to grow in importance for drug discovery. Recent developments in deep learning suggests further improvements may be gained in the analysis of large chemical data sets. It’s anticipated that neural networks will be more widely used in drug discovery in the future, and applied in non-traditional areas such as drug delivery systems, biologically compatible materials, and regenerative medicine.

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Keywords

Deep learning, neural network ensembles, neural networks, overfitting, structure-activity relationships