Predicting toxicity properties through machine learning

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Abstract

It is currently known that the high power of a drug does not fully determine its efficacy. Several properties must also be considered, including absorption, distribution, metabolism, excretion and toxicity [8]. These are the ADME-Tox properties, which are fundamental in the discovery of new effective and safe drugs. Since ignoring these properties is the main cause of failure in the development of new drugs, it is understandable that some techniques arise, such as machine learning, which apply some predictor variables as molecular characteristics to obtain models to determine some of these ADME-Tox properties. In silico models are booming because of the exorbitant expenses involved in discovering a new drug using traditional trial-and-error methods [2], and they have proven to be an effective approach to increase efficiency in drug discovery and development processes. The objective of this study is to analyze the best current machine learning techniques for predicting toxicity as an ADME-Tox property.

Palabras clave

Supervised, unsupervised learning machines, support vector machine (SVM), artificial neural networks (ANN).