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Abstract

In this article, we review recent developments in the prediction of Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) properties by Quantitative Structure – Activity Relationships (QSAR). We consider advances in statistical modelling techniques, molecular descriptors and the sets of data used for model building and changes in the way in which predictive ADMET models are being applied in drug discovery. We also discuss the current challenges that remain to be addressed. While there has been progress in the adoption of non-linear modelling techniques such as Support Vector Machines (SVM) and Bayesian Neural Networks (BNNs), the full advantages of these "machine learning" techniques cannot be realised without further developments in molecular descriptors and availability of large, high-quality datasets. The largest pharmaceutical companies have developed large in-house databases containing consistently measured compound properties. However, these data are not yet available in the public domain and many models are still based on small "historical" datasets taken from the literature. Probably, the largest remaining challenge is the full integration of predictive ADMET modelling in the drug discovery process. Until *in silico* models are applied to make effective decisions in a multi-parameter optimisation process, the full value they could bring will not be realised.

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