

This article was published in J. Comp. Aided Mol. Design (DOI 10.1007/s10822-010-9388-7) and discusses a critical issue that the community needs to address in order to use the predictive models that we build to the greatest effect.

Abstract

When we build a predictive model of a drug property we rigorously assess its predictive accuracy, but we are rarely able to address the most important question, “How useful will the model be in making a decision in a practical context?” To answer this requires an understanding of the prior probability distribution (“the prior”) and hence prevalence of negative outcomes due to the property being assessed. In this perspective, we illustrate the importance of the prior to assess the utility of a model in different contexts: to select or eliminate compounds, to prioritise compounds for further investigation using more expensive screens, or to combine models for different properties to select compounds with a balance of properties. In all three contexts, a better understanding of the prior probabilities of adverse events due to key factors will improve our ability to make good decisions in drug discovery, finding higher quality molecules more efficiently.

The full article can be accessed on-line via the Springer website at <http://www.springerlink.com/content/x15h763770611316/>

or you can

[download a preprint](#)