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### Abstract

ADMET models, whether *in silico* or *in vitro*, are commonly used to 'profile' molecules, to identify potential liabilities or filter out molecules expected to have undesirable properties. While useful, this is the most basic application of such models. Here we will demonstrate how models may be used to go 'beyond profiling' to guide key decisions in drug discovery. For example, selection of chemical series to focus resources with confidence or design of improved molecules targeting structural modifications to improve key properties....

To prioritise molecules and chemical series, the success criteria for properties and their relative importance to a project's objective must be defined. Data from models (experimental or predicted) may then be used to assess each molecule's balance of properties against those requirements. However, to make decisions with confidence, the uncertainties in all of the data must also be considered. *In silico* models encode information regarding the relationship between molecular structure and properties. This is used to predict the property value of a novel molecule. However, further interpretation can yield information on the contributions of different groups in a molecule to the property and the sensitivity of the property to structural changes. Visualising this information can guide the redesign process. In this article we describe methods to achieve these goals and drive drug discovery decisions and illustrate the results with practical examples.

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