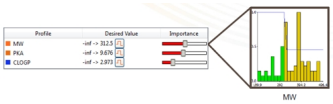
Matt Segall gave this presentation at the ACS Fall 2014 National Meeting & Exposition held in San Francisco, USA on 10th August 2014.

Abstract

In silico models are widely used in drug discovery to predict key ADME properties for compounds before synthesis or testing in *in vitro* assays. Common models cover a wide range of endpoints including physicochemical properties, absorption, blood-brain barrier penetration and interactions with proteins including enzymes, transporters and ion channels. Complex *in vivo* endpoints, such as pharmacokinetic parameters or toxicity, are more challenging to predict confidently from compound structure because they arise from multiple mechanisms, each with their own structure-activity relationships. However, in cases where we can't confidently predict an outcome, it is still possible to identify compounds with an improved chance of achieving a good result for these objectives. We will describe how predictions of multiple, relatively simple compound properties can be combined in a multi-parameter optimisation framework to target compounds with an improved chance of success against complex *in vivo* endpoints. We will illustrate how property profiles can be derived for PK and toxicity objectives and applied in the context of drug discovery.



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