Ed Champness gave this presentation at the ACS Spring 2014 National Meeting & Exposition held in Dallas, USA on 16th March 2014.

Abstract

Multi-parameter optimisation (MPO) has been widely adopted in drug discovery, to quickly target compounds with a balance of properties required for downstream success, including: potency against the intended target; absorption, distribution, metabolism and excretion (ADME) properties; and a reduced risk of toxicity. However, the increasing complexity of experimental data and calculated properties considered, even in early drug discovery, raises a challenge to determine the best profile with which to select compounds with a high chance of downstream success. We will describe recent developments that enable project teams to find and validate MPO profiles to identify the most important data and optimal selection criteria, with which to identify high quality compounds for their objectives. This enables synthetic and experimental resources to be prioritised to generate the most relevant compounds and data. We will illustrate this with example applications, including the selection of non-toxic compounds based on high dimensional *in vitro* assay data..

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