

Multi-parameter Optimisation in Drug Discovery:

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Matt gave this presentation at ELRIG Drug Discovery 2011.

Abstract

A high quality drug must exhibit a balance of many properties, including potency, ADME and safety. Identifying an optimal solution that balances multiple factors is known as 'multi-parameter optimisation' (MPO). In drug discovery this is particularly challenging due to complex, often conflicting property requirements combined with uncertain data because of experimental variability or predictive error. These make it difficult to decide with confidence which lines of enquiry to pursue and which compounds to prioritise. We will review recent developments in MPO to guide decision-making during hit-to-lead and lead optimisation. We will present a flexible approach that allows project-specific property criteria and their weights to be easily defined and integrates the available data to provide an overall compound score, explicitly taking uncertainty into account. These scores can be used to prioritise compounds with the highest chance of success while mitigating risk by exploring a diverse range of possible chemistries.

These are the slides that Matt presented.

A copy of Matt's slides is available as a [PDF](#) file.