

## Finding Multi-parameter Rules for Successful Optimization

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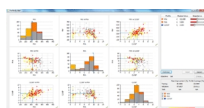
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Matt gave this presentation at the ACS National Spring Meeting 2013 in New Orleans.

### Abstract

Multi-parameter optimization (MPO) is increasingly used in drug discovery to prioritise compounds against a profile of properties required to succeed. But, how do we know what profile to use? The property criteria will depend on the ultimate objective of the project and are typically based on the subjective opinion of the project team.

In this presentation we will describe computational approaches, described as rule induction, that guide this process by analysing historical data. These identify objective multi-parameter rules that distinguish successful compounds for a chosen objective, e.g. efficacy, pharmacokinetics or safety. The resulting rules are interpretable and modifiable, allowing experts to understand and adjust them based on their knowledge of the underlying biology and chemistry. Furthermore, the importance of each criterion can be identified, allowing the most critical data to be prioritised in order to make effective compound prioritisation decisions.



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These are the slides that Matt presented.

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