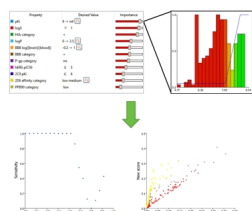


We've just submitted this article that describes how we can consider the impact of the compound selection criteria we choose on the decisions we make. Identifying sensitive criteria can highlight new avenues for exploration and potential missed opportunities.



Abstract

Drug discovery is a multi-parameter optimisation process, in which the goal of a project is to identify compounds that meet multiple property criteria required to achieve a therapeutic objective. However, having chosen a profile of property criteria, their impact on the decisions made regarding progression of compounds or chemical series should be carefully considered. In some cases, the decision will be very sensitive to a specific property criterion and such a criterion may be artificially distorting the direction of the project; any uncertainty in the 'correct' value or the importance of this criterion may lead to valuable opportunities being missed. In this paper, we will describe a method for analysing the sensitivity of the prioritisation of compounds to a multi-parameter profile of property criteria. We show how the results can be easily interpreted and illustrate how this analysis can highlight new avenues for exploration.

You can download a copy of this article as a [PDF](#) and the accompanying [Supporting Information](#).