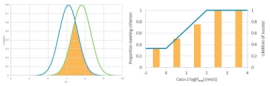
We've recently submitted this paper on the challenges of using uncertain experimental data to make confident decisions on the selection of compounds. We consider how the uncertainties in data can be translated into probabilities, when choosing between compounds or making selections based on property criteria, to avoid making inappropriate decisions, wasting effort and missing valuable opportunities.



Abstract

All of the experimental compound data with which we work have significant uncertainties due to variability in experimental conditions and the imperfect correlations between experimental systems and the ultimate in vivo properties of compounds. When using these data to make decisions, it is essential that these uncertainties are taken into account to avoid making inappropriate decisions in the selection of compounds, which can lead to wasted effort and missed opportunities. In this paper we will consider approaches to rigorously account for uncertainties when choosing between compounds or selecting compounds against property criteria; first for an individual measurement of a single property and then for multiple measurements of a property for the same compound. We will then explore how uncertainties in multiple properties can be combined when assessing compounds against a profile of criteria, a process known as multi-parameter optimisation. This guides rigorous decision-making using complex, uncertain data to focus on compounds with the best chance of success, while avoiding missed opportunities by inappropriately rejecting compounds.

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