Abstract:

Computational tools can guide the selection of high quality compounds, with a good balance across multiple properties, and guide strategies to design improved compounds. But, can software propose ideas for better compounds? We will demonstrate an approach that generates compound ideas and identifies those that are most likely to achieve a drug discovery project’s objectives. The compound ideas should be synthetically feasible; to achieve this, new structures are generated from an initial compound using medicinal chemistry ‘rules’. These are then scored against a profile of property criteria using a probabilistic scoring method and visualized in ‘chemical space’ to allow many ideas to be rapidly explored and prioritized for detailed consideration.

In this poster we will demonstrate an approach that generates compound ideas and prioritises those that are most likely to succeed against a drug discovery project’s objectives. The goal is to stimulate the search for high quality compounds by helping to explore a diverse range of strategies and highlight the best for detailed consideration.

A copy of this poster as available as a [PDF].
ways to improve productivity and restore the rate of successful drug launches; however with help to overcome these psychological barriers, better decision-making can enhance R&D performance [1].

We will discuss four of the common biases that have serious implications for decision-making in drug discovery (summarised below). We will suggest approaches for overcoming these, such as strategies adapted from evidence-based medicine and computational tools that seek to guide the decision-making process, encouraging objective consideration of all of the available information and explicit consideration of the impact of uncertainty in drug discovery.