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Abstract

A plethora of cheminformatics approaches have been developed to support drug discovery. These include methods for: analysis of structure-activity relationships (SAR), such as matched molecular pair analysis (MMPA), activity cliff detection and R-group decomposition; prediction of properties, including potency, physicochemical and absorption, distribution, metabolism and excretion (ADME), using quantitative structure-activities (QSAR) models; integration of data from public domain and proprietary sources; multi-parameter optimisation to identify high quality compounds with a balance of the properties required for success; and selection of compounds, considering both quality and diversity to avoid missed opportunities.

No single method is likely to provide a solution to the challenges of drug discovery. However, judicious use of cheminformatics 'tools', used in combination, can make a significant difference to the productivity and efficiency of drug discovery. One approach is to link multiple cheminformatics algorithms in a 'pipeline', but this can limit the ability of the medicinal chemist to interact with the process. Instead, seamless integration of methods in an intuitive and highly visual environment can maximise the synergy between the expert chemist’s knowledge and the algorithms’ abilities to process complex data.

In this presentation, we will provide some illustrative examples of workflows addressing challenges at different stages of the drug discovery process. We will demonstrate, through practical case studies, how such approaches can quickly target high quality compounds, reducing the time and resources required to find high quality lead and candidate compounds.

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