This poster by Matthew Segall[1], Tamsin Mansley[1], Peter Hunt[1], Kelly Chibale[2], Tanya Paquet[2], James Duffy
[3]

was presented at the RSC Cambridge Medicinal Chemistry Meeting held in Cambridge, UK.

Abstract

The not-for-profit and academic sectors have become important sources of novel drug candidates, particularly for neglected and developing world diseases or niche indications. Drug discovery projects in these sectors are often conducted on a collaborative basis, pooling resources and experience across multiple research groups and using contract research organisations as appropriate. Several software platforms have been developed to facilitate the secure sharing of data across organisations, but in this talk we will discuss software approaches that focus on using these data to guide decisions regarding the selection and design of high quality compounds.

Given the limitations of the resources available to projects in these sectors, it important to quickly focus on chemical series and leads with the best possible chance of success downstream. Enabling this requires a combination of capabilities including visualisation and analysis of project data, interpretation of structure-activity relationships and predictive modelling to guide the design of new compounds for synthesis and testing. In this talk, we will describe the underlying methods and illustrate how they can be linked to platforms for sharing of data, to facilitate collaborative approaches to drug optimisation.

We will illustrate the approaches described in this talk with an application to a drug discovery project targeting malaria. We will demonstrate how an integrated application of computational approaches can help to guide the multi-parameter optimisation of efficacy against drug sensitive and resistant strains of plasmodium parasites, as well as absorption, distribution, metabolism, excretion and toxicity (ADMET) properties.

You can download this presentation as a PDF .