

Exploring the chemical space of screening results

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Monday, 29 April 2013 00:00 - Last Updated Thursday, 17 October 2013 14:57

Ed Champness gave this presentation at the ACS National Spring Meeting 2013.

Abstract

When faced with the results from a screening campaign it is essential use this data to quickly focus on the best chemistries for progression. In this presentation we will describe two techniques for visualising a 'chemical space' to guide this exploration. We will demonstrate how these can be used to identify activity 'hotspots' and focus on these for detailed analysis of structure-activity relationships. This approach can also help to spot singletons and outliers that may represent false positives or negatives for further investigation. Furthermore, it is well understood that high quality chemistry will have not only good activity, but also appropriate absorption, distribution, metabolism, elimination and toxicity (ADMET) properties. We will show how data from multiple sources can be combined to select compounds for further study with an appropriate balance of activity, ADMET properties and structural diversity to mitigate downstream risk.

These are the slides that Ed presented.

A copy of Ed's slides is available as a [PDF](#) file.