Matt gave this presentation at the ACS National Fall Meeting 2012.

## Abstract

Many approaches have been used to characterise compounds as 'drug-like' or not based on the similarity of simple properties of a compound, e.g. molecular weight, to those of known drugs. However, having a 'similar' property to known drugs does not necessarily mean that a compound is more likely to become a drug. We propose an extension to 'drug likeness' approaches, based on an assertion that a desirable value of a property is one that increases the probability of identifying a drug. Using Bayesian approaches we can estimate the relative likelihood of a compound being a drug by comparing the distributions of properties for drugs and non-drugs. We will demonstrate that this offers improved performance for the identification of drugs and provides insights into which characteristics provide the greatest discrimination between successful drugs and unsuccessful drug discovery compounds.

These are the slides that Matt presented.

A copy of Matt's slides is available as a PDF file.