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

Abstract

We will explore the accuracy of current computational methods in drug discovery, including 2D and 3D QSAR, docking, pharmacophore, molecular dynamics and quantum mechanical approaches. Based on this, we will address the question of whether we are truly operating in a drug design paradigm. We will compare this with the application of computational methods to the discovery of new drugs. From this alternative perspective, computational methods can add significant value to guide decisions about which chemistry to pursue and which can be rejected with confidence; focussing resources on the chemistry that is most likely to succeed, while avoiding missed opportunities. This is particularly important in the multi-parameter optimisation of high quality drug candidates that require a balance of many properties to succeed downstream.

These are the slides that Matt presented.

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