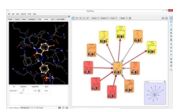


Tamsin Mansley gave this presentation at the ACS Spring National Meeting & Exposition held in San Diego, USA on 13th March 2016.

Abstract

Chemists frequently draw upon their experience and chemical intuition to make sense of complex project data and select new compounds to synthesize. However, drug discovery projects increasingly demand greater efficiencies with shorter timelines and lower costs, putting medicinal chemists under pressure. Additionally, the traditional divide between computational modellers and synthetic chemists is no longer clear and software must be easily accessible across disciplines; project teams need to quickly understand and predict structure-activity relationships (SAR), identify potential liabilities and design new compounds with the highest chance of success.



Multi-parameter optimisation (MPO) approaches help to bring together complex data, quickly and objectively targeting high quality compounds, while visual analyses such as activity cliff detection and matched pair/series analysis, enable rapid evaluation and exploitation of structure-activity relationships (SAR). At the same time, the ability to consider these 2-dimensional (2D) analyses alongside 3-dimensional (3D) structure-based information ensures that all available evidence is applied to the design of new compounds. Furthermore, when considering the next round of synthesis, predictive models can guide the design and selection of new compounds to improve properties and activity. However, providing all of these capabilities within a single environment requires a delicate balance; it is critical to ensure that the capabilities are comprehensive and rigorous while being easily accessible to all.

In this talk we described new methods that guide compound selection and design, brought together in an intuitive interface within which a chemist can bring their own experience to bear. We illustrated these with case studies that demonstrate how this enables new strategies for compound optimization that reduce the number of design-synthesis-test iterations in a project, saving time and reducing costs. .

You can download this presentation as a [PDF](#) .