In this webinar, held on 13 December 2017, Juliette Pradon, of Cambridge Crystallographic Data Centre describes the science behind the GOLD docking platform and Matt Segall demonstrates the link between StarDrop and GOLD, combining 2D and 3D SAR to guide the design of high quality compounds.

Abstract

Protein-ligand docking allows the binding mode and conformation of a molecule within a protein active site to be rapidly explored *in silico*. Within a drug discovery project, docking can be applied to rationally design new and modify existing ligands, as well as to search through a database of hundreds of thousands of molecules for potential hits. The docking outcomes are usually improved when you are able to include known information about the protein-ligand system in the docking process. This may be achieved through the use of constraints to ensure, for example, that key H-bond interactions are fulfilled, or to bias docking results towards a known binding motif. Where there are several existing structures for the target of interest, which may involve protein backbone movement as well as sidechain movement, and you are not sure which is the best model to select, an ensemble docking approach can prove useful.

We finish with a brief demonstration of how StarDrop can be seamlessly interfaced with GOLD. This enables multiple iterations of design in 3D in real time, linked with StarDrop's data visualisation, 2D SAR analyses and predictive models.

To hear the narration, please increase your speaker volume.