In this webinar, held on 6 April 2016, Marcus Gastreich of BioSolveIT described the technology underlying their HYDE scoring function and SeeSAR. This also included worked examples to demonstrate how visually informed lead optimisation can save you considerable time, leading to compounds with an improved profile.

To hear the narration, please increase your speaker volume.

"Seeing is believing", people say. Too often though, computers leave us feeling that we have to believe without seeing: A number is delivered by an algorithm and experts are required to interpret the results or the research team is expected to believe in this - or not.

SeeSAR™ is a structure-based design tool which breaks this ‘take it or leave it’ mould, providing medicinal chemists with an interactive means to interpret 3D structure-activity relationships (SAR). Combining affinity estimates, taking desolvation and entropic factors into account, with statistical analysis of torsions, SeeSAR takes a highly visual approach to exploring 3D SAR, so that compounds can be quickly prioritised and evolved.