M. Gastreich[1]

STAYING CRITICAL ALL THE WAY: WHERE TO PAY EXTRA ATTENTION IN LEAD GENERATION AND OPTIMIZATION

[1] BioSolveIT, Germany

When we start a structure-based project, there are many pitfalls along the way: Crystallographic uncertainties, tautomer selection, protonation variations, duplicates in molecular files, and so on. The tutorial will help sharpen the view for the typical pitfalls - and give software assistance to detect and deal with them.

Beyond data preparation and handling there is the ubiquitous question of WHERE a ligand binds and HOW STRONG the association is compared to the unbound state, i.e., the affinity estimation.

Using SeeSAR, a very new tool from BioSolveIT, we will visualize and discuss critical cases and see how to improve compounds. We will concentrate about WHAT affinity really is and what it drives, and we will get a deeper insight into the way how esp. Medicinal Chemists, our closest partners in drug hunting, think when they look at protein-ligand complexes.