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A tale of a low molecular weight inhibitor for Bruton's Tyrosine Kinase, modeled in SeeSAR, the world's best compound ideation software for medicinal chemists

In this workshop, we will showcase the most important features to get you going with SeeSAR, the easy-to-use software for medical chemists. We will use an example published by Takeda, in which they described the discovery new inhibitor for Bruton's Tyrosine Kinase, Btk, which is of lower weight than ibrutinib and also doesn't bind covalently against the target. The workshop will walk you through analyzing the protein-ligand complex and the details of editing the ligand starting from the crystal structure until we arrive at the published structure. By means of the editing process, all important features of SeeSAR will be explained in great detail, so that participants will be able to start doing their own compound ideation after the workshop. A free license will be provided in succession of the workshop.

Biography

Carsten Detering obtained his PhD in Physical Chemistry from the Freie Universitaet Berlin in Germany in 2001. He did his Post Doc at the University of Washington in Seattle where he worked on the application of docking software for nucleic acid drug targets and rational design of new inhibitors for a malaria project. In 2005 he came to BioSolveIT in Germany as an Application Scientist first, later filling the position of Senior Key Account Manager and Executive VP of Sales, North America, before moving back to Seattle as CEO of BioSolveIT Inc, the North American subsidiary of BioSolveIT.

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