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Visual binding: A radically new concept to support the medicinal chemist's quest for innovative NMEs

Carsten Detering
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The introduced next generation of binding affinity assessment tool Hyde, has been incorporated into a new software, SeeSAR, which helps the medicinal chemist assess, modify and prioritize compounds within the context of the protein. Hyde has been completely revamped and shows another huge step forward to accurate compound scoring. After having optimized the protein-ligand complex, Hyde accounts for the hydrogen bond and desolvation energy of a ligand binding to a protein, effectively ruling out false positives by incorporating penalties for unmet interactions. Those penalties are visually communicated, giving intuitive clues where to improve the molecule with respect to binding affinity. An interactive editor helps making the necessary modifications, and the scientist gets immediate feedback whether those changes are leading into the right direction, i.e. if the binding affinity is getting better or not. The talk will highlight the science behind Hyde as well as case studies which demonstrate Hyde's effectiveness.

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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