Carsten Detering, Med chem 2015, 5:10
http://dx.doi.org/10.4172/2161-0444.C1.014

OMICS International
conferenceseries.com
4th International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
November 02-04, 2015 Atlanta, USA

Carsten Detering
BioSolveIT Inc., USA

Bridging the Dimensions: How 2D Structure-activity Relationships and 3D Structural Binding Affinity help to Guide Medicinal Chemistry

The borders between traditional medicinal chemists and computational chemists have been blurred in the past 10 years. Medicinal chemists today are much more likely to assume more and more computational tasks. This entails crafting more intuitive software from the software industry, and also the seamless integration of 2D SAR data with 3D structural information to combine the medicinal chemist's view of things with that of the computational chemist.

This talk will highlight how we can utilize information from 2D ADME/T property models and 3D views of protein-ligand complexes. A glimpse into the near future will show, how the influence of each atom or functional group on these properties can be highlighted and combined with visualization of the atomistic contributions to binding affinity.This enables development of optimization strategies that balance potency with the ADMET properties required in a safe and efficacious drug, thus giving this phase of the pipeline more efficiency by means of a truly multi-parameter optimization environment.

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.

detering@biosolveit.com

Notes: