Carsten Detering, Med chem 2015, 5:10
http://dx.doi.org/10.4172/2161-0444.C1.015

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

How close are we to predicting binding affinity?

Carsten Detering
BioSolveIT Inc., USA

Predicting binding affinity (aka scoring a protein-ligand complex) has been heavily criticized as long as it exists. Sometimes it works on this target, sometimes on another target, but there are few, if any that work consistently well on all targets. One possible explanation and certainly a drawback could be that existing ways of predicting binding affinity (scoring functions) look at favorable interactions, neglecting those interactions that are unmet, which consequently brings into a virtual screening a lot of false positives. BioSolveIT's scoring function Hyde takes on these challenges and is radically different. It is based on pure physico-chemical principles and takes into account hydrogen bonding and the hydrophobic effect. It penalizes missing interactions, wherever a hydrogen bond is not established or a group is misplaced in the active site. This effectively rules out most false positives. There are cases, however where there is hardly coincidence between the experimental and the calculated affinity. Does this mean Hyde does not work as reliably as we expect? We will look at some examples and check who we should trust: our crystal structures or the Hyde scoring function.

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

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