

3rd International Conference on Medicinal Chemistry & Computer Aided Drug Designing

December 08-10, 2014 DoubleTree by Hilton Hotel San Francisco Airport, USA

New developments in docking and scoring

Istvan J Enyedy¹ and Mark Mc Gann² ¹Biogen Idec, USA ²OpenEye Scientific, USA

Over the last two years, we have set up about 300 internal structures and more than 10,000 compounds for testing docking and scoring strategies. We used this set for evaluating the new scoring function CHEMGAUSS5 implemented into FRED and HYBRID from OpenEye. The presentation will show the improvements that obtained using the latest scoring function when compared to CHEMGAUSS4, the correlation of a few components of the scoring function with IC50, the impact of using information from solvent mapping to guide docking, and recommended statistical analysis for estimating errors in docking runs.

Biography

Istvan J Enyedy has been involved in new target evaluation, hit finding, and hit-to-lead optimization projects for proteins from several target classes using both ligand and structure-based methods. He is coauthor of more than 30 publications and 11 patents/applications. He received his PhD in 1998 at Catholic University of America, Washington DC, and did postdoctoral training in Dr. Shaomeng Wang's group at Georgetown University Medical Center, Washington DC. Between 2001 and 2008, he worked at Bayer Pharmaceuticals, West Haven CT and Novartis Institutes for Biomedical Research in Cambridge MA. Since August 2008, he has been working at Biogen Idec, in Cambridge MA.

istvan.enyedy@biogenidec.com