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New approaches to "Hit" optimization

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Abstract

Target structure-based "hit" optimization in a drug discovery project is challenging from the computational point of view. Scoring functions cannot predict binding affinity, thus computational chemists must use their intuition or prior knowledge about the target class to prioritize compounds for synthesis. As the pharmaceutical industry targets novel protein classes, computational chemists must use software to build their know-how about the protein. The talk will focus on how we can use solvent mapping and information from cocrystal structures in guiding docking and scoring. Test results of this procedure on seven kinases using the HYBRID docking protocol from OpenEye will be shown.

Biography

In the past 14 years Istvan J Enyedy has been involved in new target evaluation, hit finding, and hit-to-lead optimization projects for several types of target classes using both ligand and structure-based methods. He is coauthor on more than 30 publications and 9 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.