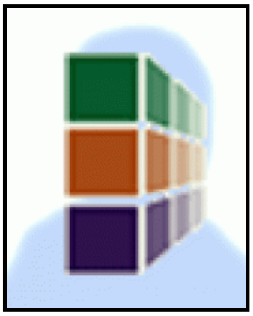

Special Guest Lectures

Ligand Homology Modeling as a new computational platform to support modern drug discovery

Michal Brylinski, Georgia Institute of Technology, Atlanta

Research Scientist II, Center for the Study of Systems Biology

Johnston Hall 338
May 10, 2011 - 10:00 am

Abstract:
As an integral part of drug development, high-throughput virtual screening is a widely used tool that could in principle significantly reduce the cost and time needed to discover new pharmaceuticals. In practice, virtual screening algorithms suffer from a number of limitations and the development of new methodologies is required. In this talk, I will discuss the ideas of Ligand Homology Modeling (LHM), which is likely one of the first approaches in Cheminformatics that successfully extends template-based techniques, commonly used in proteins structure prediction, to the modeling of protein-ligand interactions. Our intensive research in this field culminated in the development of a novel virtual screening approach, which appears as a powerful compound prioritization technique applicable to the early stages of proteome-scale drug design projects. As an example, I will describe the application of LHM to all kinase domains in humans, which has provided the scientific community with a very extensive structural and functional characterization of the human kinome to support the discovery of novel kinase inhibitors.

Speaker's Bio:
Michal Brylinski currently works at the Center for the Study of Systems Biology, Georgia Institute of Technology, as a senior research scientist. Brylinski received his Ph.D. in Chemistry from Jagiellonian University, Krakow, Poland (2006); and his M.S. in Pharmacy from Wroclaw Medical University, Poland (2000). His research interests are: systems biology, chemical systems biology and cheminformatics; drug discovery and design; low-resolution ligand docking; ligand comparative modeling; protein function inference; protein structure prediction; protein evolution; and engineering and simulation of life.

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