Computational Biology Seminar Series for Undergraduates

Computational Biology, Drug Discovery and Xbox 360

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Life Sciences Building Annex A101
October 07, 2013 - 05:30 pm

Abstract:

To speed up the development of new biopharmaceuticals, computational approaches for the identification of lead compounds are widely used. In particular, virtual screening is becoming an integral part of modern drug development pipelines. Due to advances in computer technology resulting in constantly increasing computational power, virtual libraries comprising millions of compounds can be rapidly evaluated in silico prior to experimental screens and at a fraction of the cost. Here, the idea is to considerably reduce the number of candidate compounds that need to be tested experimentally. In this talk, I will discuss computational biology tools that are commonly used in modern drug discovery. As an example, I will walk through a computational study focusing on the development of novel antibiotics against acetyl-CoA carboxylase, which is part of a multi-disciplinary drug design project recently started at LSU. Finally, I will talk about how cutting-edge computer technology developed primarily for video game industry can be used to support scientific research as well, including the discovery of new drugs.

Speaker's Bio:

Michal Brylinski is an assistant professor in the Department of Biological Sciences and the Center for Computation & Technology at LSU. A pharmacist by training, he decided to maneuver his career towards computational aspects of drug discovery and design. After obtaining a Ph.D. in Chemistry from Jagiellonian University in 2006, he spent two years as a postdoc in a computational biology lab at Georgia Tech. He continued his research at Tech as a Research Scientist till 2012, when he joined LSU. His current research combines chemical systems biology, structural bioinformatics and cheminformatics with high-performance and heterogeneous computing, with applications to modern computer-aided drug development. He is an author of 46 publications, 3 of which were featured on journal covers of Proteins, Journal of Chemical Information and Modeling, and Physical Chemistry Chemical Physics. He serves as a reviewer for over a dozen of scientific journals and as an editor for Bio-Algorithms and Med-Systems. As a member of statewide LONI Institute and LA-SiGMA, he enjoys working on interdisciplinary projects with undergraduate and graduate students from Biology, Physics, Chemistry, Computer Science and Electrical Engineering. Visit http://brylinski.cct.lsu.edu for details.

This lecture has refreshments @ 05:00 pm
This lecture has a reception @ 05:00 pm