Computational Biology Seminar Series for Undergraduates

What's Up Doc(k)?

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Life Sciences Building Annex A101
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Abstract:

I will present recent advances in technology and applications of computational docking, a computational biology approach that aims at identifying small molecules that can bind to protein targets. This approach has been for instance used for quite some time in the pharmaceutical industry to discover new potential drugs. Recent supercomputers promise to revolutionize docking by allowing very complex problems to be tackled, but the associated fundamental and technical challenges are important.

Speaker's Bio:

Professor Jerome Baudry joined the Center for Molecular Biophysics in 2008 as an Assistant Professor at the University of Tennessee, Knoxville; Department of Biochemistry & Cell and Molecular Biology. Dr Baudry obtained his Ph.D. in Molecular Biophysics with the highest Honors from the University of Paris-06, France (University Pierre and Marie Curie). He subsequently joined the group of Klaus Schulten at the University of Illinois at Urbana-Champaign as a post-doc. After his post-doctoral work, Dr. Baudry worked in the pharmaceutical industry as a Research Scientist, and then accepted a Senior Research Scientist position back in Illinois. Prior to his appointment in Tennessee, Dr. Baudry was Research Assistant Professor in the School of Chemical Sciences at the University of Illinois, Urbana-Champaign.

The Baudry laboratory develops and applies methods and protocols in computational molecular biophysics for structure-based molecular discovery. The lab works on several targets relevant to human and animal health as well as on targets of agrochemical interest. The theoretical approach is complemented by close collaborations with experimental groups. The Baudry lab also actively pursues research projects to characterize the role of methyl-rich side chains in the dynamics and the thermodynamics of protein/protein and protein/ligand interactions. This has led the group to further develop frontier projects on the dynamics of satellite functionalization in solid state, and surface-mounted nano rotors.

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