CCIB Annual Retreat 2014

Waterfront Technology Center
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Presentation Abstracts

Hao Zhu

Cheminformatics has been defined as the science of examining the structure and function of chemicals through the use of computational analysis, statistics, and pattern recognition. A number of recent workforce studies have shown that there is a high current and unmet demand for people trained to various levels of expertise in informatics, from technicians and technical librarians to developers of new and improved methodologies and applications. Dr. Zhu's lab is using the cheminformatics algorithms, workflows and other relevant computational tools to model chemical toxicity, ADME (Absorption, Distribution, Metabolism and Excretion) and other biological activities. The resulting models will be used in the regulatory chemical toxicity assessments and the CADD (Computer-Aided Drug Discovery) process.

Eric Klein

The dynamic regulation of virulence is an essential aspect of pathogenesis that holds great promise for combating infectious disease. While the overwhelming emphasis of the field to date has been on the chemical cues that mediate bacteria-host interactions, there is evidence indicating that bacteria can also sense and respond to their mechanical environment. In particular, I have demonstrated that uropathogenic *Escherichia coli* (UPEC) induce a novel gene expression program in response to adhesion to stiff surfaces. While the mechanism by which fimbriae attach to their targets is well understood, little is known about how fimbrial attachment may trigger pathogenic gene expression. Using a variety of genetic and microscopy-based approaches, my work will focus on how mechanical forces stimulate adhesion-mediated gene expression, the mechanism of bacterial mechanotransduction, and the role of mechanical signaling in pathogenic infection. Ultimately, my goal is to identify components of the mechanotransduction pathway as targets for the development of novel therapeutics for use as alternatives to traditional antibiotics.

Jongmin Nam

We study how differential gene expression patterns are established and maintained in developing embryos. We also develop new experimental tools and analytical tools for high-throughput cis-regulatory analysis in embryos and cells. We are open for collaboration on any topics related to gene regulation and evolution.

Grace Brannigan

Research in the Brannigan group focuses on computational studies of neuronal proteins and their interactions with lipids, endogenous hormones, and drugs acting on the central nervous system. Large-scale Molecular Dynamics calculations conducted on high performance computers are used to investigate the effect of single nucleotide polymorphisms (SNPs) on protein dynamics, as well as to elucidate the molecular mechanisms underlying actions of anesthetics, thyroid hormone, and neurosteroids. Sophisticated free energy calculations yield quantitative characterizations of binding affinities and conformational change. We are interested in collaborations with both experimentalists and theorists; our techniques are most suitable to investigations involving one to three proteins of known structure.

Desmond Lun

The Lun Lab has expertise in systems biology and computational biology. In particular, we work on whole cell and pathway modeling, with emphasis on metabolism and the application of modeling to metabolic engineering. We also work on analysis of biological data, including sequencing data, forensic DNA markers, expression data, and metabolomic and fluxomic data.

Min Kyung Kim

Prediction of internal metabolic fluxes of microorganisms is important to understand intracellular mechanisms of their metabolic responses as well as to identify molecular targets for the metabolic engineering. By integrating microbes' *in silico* models with transcriptomic data, we've developed a computational method that can predict internal metabolic fluxes in an efficient way. We've examined *E.coli* and *S.cerevisiae* first as our model species, and the algorithm's predictive accuracy was validated by calculating correlation with *in vitro* flux measurement data. We're planning to apply this method to analyze systemic metabolic networks of other species.

Andrey Grigoriev

Our group pursues computational genomic analyses in various biological fields, from cold microbiomes to small RNA function to genome rearrangements.

Dan Shain

Research interests: Annelid development and evolution

Current research areas:

1. Cloning and expression of genes differentially expressed during stem cell formation.
2. Genetic and ultrastructural analyses of leech cocoons
3. Bioenergetics of ice worms and extremophilic microbiota.
4. Ice worm phylogeny and phylogeography.

Kwangwon Lee

Because of its relative simplicity and the rich knowledge that has accumulated over many years, Neurospora is an excellent model system for studying complex biological phenomena such as the circadian clock. A half-century of Neurospora circadian clock research have contributed significantly to our understanding of the molecular structure of the circadian oscillators in higher organisms, including humans. However it has been difficult to gain a comprehensive understanding of how the circadian clock works due to its complex nature and technical obstacles. The long-term goal of my laboratory is to understand how complex circadian rhythm behavior is controlled at the molecular level. Currently, we are working on identifying/characterizing novel clock genes using natural isolates and mapping populations. The outcome of our research will reveal novel insights on the eukaryotic circadian system at the genetic and molecular level.

Catherine Yang

My research programs are primarily focused on the molecular recognition in various biological systems, proteolytic regulatory roles, particularly in diabetes and cancer area. We have designed a series of DPPIV inhibitors which exhibit promising potencies, and we are in the process of refining our target model. This finding has resulted in an intellectual property filed as a US Patent. Preclinical and molecular modeling expertise would be synergetic. We are also interested in another protease target in regulating prostate cancer progression whereas we discovered lead compounds in regulating the availability of insulin growth factors. Sponsored by NIH, we are continuously interested in the understanding the molecular basis of this regulatory mechanism. Development of drug analogs with higher potency can be carefully orchestrated based on the molecular modeling optimization. Biomarkers in prostate cancer for early diagnosis have been investigated. Expertise in biomedical device design is very much appreciated. In addition, we are also working on peanut allergy vaccine development joint with Dr. Coifman, a clinician from South Jersey Allergy. Expertise in immunology and animal models is complementary.

Bill Saidel

Two projects from the Laboratory of Assoc. Prof. Wm. Saidel

1. The influence of stochastic resonance on the Jamming Avoidance Reflex of weakly electric fish
with Prof. Sunil Shende, Computer Science and student Christopher Cherfane

The Jamming Avoidance Response is a neurobiological reflex in which the frequency of self-generated electric signals is changed when the electric field of a 2nd individual of the same species interacts with the field of the first individual. One raises its EOD (electric organ discharge) frequency; and the other lowers its frequency, thereby increasing the separation between the two sets of signals. We are using this reflex to test for the existence of stochastic resonance (SR) in this system. SR is a phenomenon that improves detectability of a threshold signal in the presence of noise. We are developing an autonomous Matlab based program that will simultaneously record the EOD and return to the fish both the emitted EOD at varying amplitudes coupled with an added noise signal to determine if a subthreshold EOD plus a noise signal will elicit the JAR.

2. Dynamics of starlings 'en mass'
with Dr. B. Picolli, students Scott Davis* and Bryan Gatchmo

Starlings often fly in clouds of individuals who rarely if ever collide (a 'murmuration'). The organization of the cloud appears to be an emergent property of individuals who pay attention to not more than 7 neighbors. We are exploring this notion by building a radio-controlled octocopter carrying two GoPro cameras separated by about 3.5 meters. The octocopter with its synchronized cameras will be used to fly into a flock to determine the x-, y-, and z-position of individuals within the flock and as the flock responds to the "attacking" octocopter. This data will be used to determine the dynamics of each bird's avoidance movements and to determine if individuals are coupled with neighbors as they avoid the octocopter.

*superb engineer

Joe Martin

The goal of our current research is to clarify how thyroid hormones influence the adult mammalian brain. During growth and development, hormones from the thyroid gland enter many cell types (including brain cells) and alter protein synthesis. In adulthood, the cellular metabolic rate is accelerated by thyroid hormones entering cells of many tissues, but not in the brain. However, some of the potentially most debilitating complications of thyroid glandular disease are due to neurological disorders, ranging from anxiety and sleep problems to seizures or coma. Our studies have implicated nongenomic mechanisms, including $GABA_A$ receptor function and phosphorylation of nerve terminal proteins, in the actions of thyroid hormones in adult brain. Microinjections of thyroid hormones into sleep-related brains structures have also been shown to alter sleep patterns in ways consistent with nongenomic effects of the hormones.

Recently, our interests have expanded to computational modeling of biological systems, including abstract theoretical models of brain function (with Dawei Hong), more concrete models of biological rhythms (with Benedetto Piccoli and Robi Polikar) and molecular dynamics simulations of the $GABA_A$ receptor (with Grace Brannigan).