e-Bioinformatics Workshop at IEEE e-Science '08

Friday, December 12 (9:30 am–3:30pm)
IUPUI University Conference Center & Hotel, Room 232 (see map below)

Workshop Program

Keynote

Introduction: Mehmet M. Dalkilic (Indiana University, Bloomington)

9:30-10:20pm **Bioinformatics of Intrinsically Disordered Proteins**

- Dr. A Keith Dunker
  T-K Li Professor of Medical Research, Professor of Informatics, Professor of Biochemistry and Molecular Biology, Director of Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, IN

Session I (morning)

Chair: Daisuke Kihara (Purdue, West Lafayette)

10:30-11:15pm **Cloud Computing for Bioinformatics**

- Dr. Simon Lin
  Director of Bioinformatics Consulting, Robert H. Lurie Comprehensive Cancer Center & Biomedical Informatics Center, Northwestern University, Chicago, IL

11:15-noon **Bio-computing and Knowledge Discovery of Molecular Networks**

- Dr. Jake Chen
  Assistant Professor of Informatics & Computer Science, Founding Director of Indiana Center for Systems Biology and Personalized Medicine, Indiana University – Purdue University, Indianapolis, IN

Session II (afternoon)

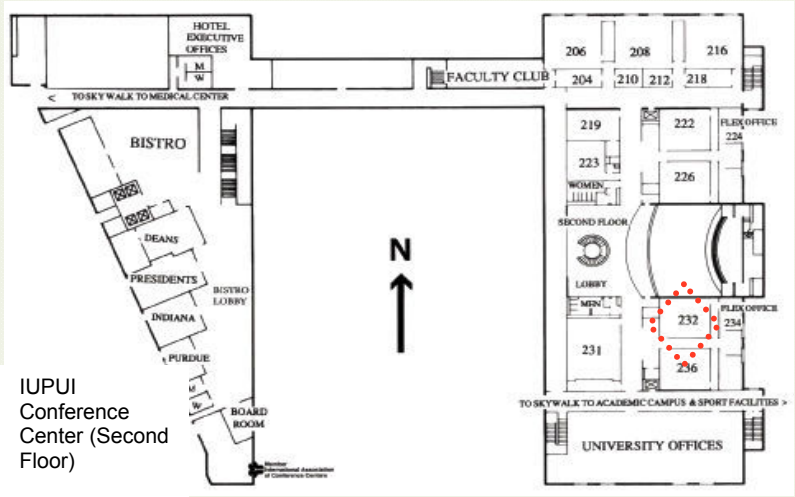
Chair: Jake Chen (IUPUI)

2:00-2:45pm **Mining Specific Protein-DNA Interactions for DNA Binding-site Prediction**

- Dr. Yaoqi Zhou
  Professor of Informatics & Biochemistry, Director of Bioinformatics Program, School of Informatics, Indiana University, Indianapolis, IN

2:45-3:30pm **Annotating Protein Structures by Surface Shape Comparison**

- Dr. Daisuke Kihara
  Assistant Professor of Computer Science & Biology, Purdue University, West Lafayette, IN



IUPUI Conference Center (Second Floor)

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Bioinformatics of Intrinsically Disordered Proteins

A. Keith Dunker

Many proteins lack specific 3-D structure and yet carry out function. Starting in 1996, we began to explore the prediction of structured and disordered regions from amino acid sequence. Disorder predictions by us and others suggest that a large fraction of eukaryotic proteins contain significant-sized regions of disorder. Recently we developed a bioinformatics approach to assign the functions in Swiss-Prot to structure (order) or to disorder. Of 710 common functions, 310 correlate with structure and 238 with disorder, but the repertoire for disorder is broader. Protein interaction networks often involve one protein binding to multiple partners. Disorder is commonly used for this purpose. In four recently reported examples, promising drug-lead molecules bind to structured proteins and thereby block their interactions with disordered partners. Study of these examples has led to a new approach to drug discovery. Protein function is frequently modulated by posttranslational modification, and these events happen far more often in disordered regions than in structured regions. Alternative splicing is very common and well developed in multicellular eukaryotes but more nascent in single-cell eukaryotes. The RNA removed by alternative splicing is found to code for intrinsic disorder significantly more often than for structure. Given that signaling segments in regions of disorder are formed from small numbers of contiguous amino acids, and given that many disordered regions have been shown to contain many signaling and regulatory segments in tandem, alternative splicing within regions of disorder provides a mechanism for bringing about regulatory and signaling diversity. We propose that alternative splicing plus intrinsic disorder, plus posttranslational modification provided a means to "try out" alternative regulatory pathways, thus facilitating the evolution of multicellular organisms.

Bio:

A. Keith Dunker received a broad education, with degrees in chemistry (UC Berkeley, 1965), physics (UW Madison, 1967), and biophysics (UW Madison, 1969), and with postdoctoral training in structural biology (1969-1973, Yale University). After spending a career using biophysics and spectroscopy to study virus and phage structure and assembly as models for understanding connections between protein conformational changes and function, in the middle 1980s Dr. Dunker realized the coming importance of computational biology and bioinformatics and began to teach, to work and especially to collaborate "on the side" in these newly developing areas. His biophysics work and his computational hobby merged in the mid 1990s with the realization that many proteins lacked 3D structure yet carried out function and could be studied as a group using bioinformatics approaches and methods. His "second career," which focuses on the bioinformatics of intrinsically disordered proteins, is leading to novel ideas regarding protein structure and function, and these will be the topics of his seminar.