biomedical and health informatics

Biomedical and Health Informatics Lecture Series

Course Website: Link

Tuesday, May 15, 2012
12:00 - 12:50 p.m., Room T-663

Valerie Daggett, PhD

Professor, Bioengineering, College of Engineering and School of Medicine
Adjunct Professor, Biochemistry Department
Adjunct and Core Professor, Biomedical and Health Informatics
University of Washington

"Dynameomics"

The goal of Dynameomics is to perform atomistic molecular dynamics (MD) simulations of representative proteins from all known folds in explicit water in their native state and along their thermal unfolding pathways. This has now been accomplished. We are now mining these rich and vast dataset and developing new mining and visualization tools geared towards discovery and use of the results for a variety of purposes. Various libraries have been created from the data for protein design and structure building. To encourage understanding of the relationships between protein dynamics, function and disease, we have constructed a web site, complementary to the PDB, which allows access to a novel hybrid relational/multidimensional database to view and interrogate simulations of the Top 100 targets: http://www.dynameomics.org. The Dynameomics database should also be useful for determining the rules governing protein folding and kinetic stability, which should aid in deciphering genomic information and for protein engineering and design. This database contains both the largest collection of protein simulations and protein structures in the world. Visual analytics is becoming increasingly important for interrogating these massive data sets and newly developed tools in the lab will be presented.

Dr. Daggett has 25 years of experience performing simulations of proteins. She developed the approach of simulating protein unfolding to characterize the folding process. She also was the first to use simulation methods to map conformational changes associated with amyloidosis. At UW she was a founding member of the Biomolecular Structure and Design Program and until recently the director. She is PI of NIH, Human Frontiers of Science, Microsoft, DOE, and NSF grants. Dr. Daggett is the Senior Editor of Protein Engineering Design and Selection (PEDS) and she is on several editorial boards: Biochemistry, Structure, and Biomedical Computation Review. She was elected a Fellow of the Biophysical Society in 2011. Dr. Daggett has published >200 scientific papers, which have garnered ~9000 citations.

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NOTE: Podcasts from MEBI 590 Lecture Series talks for this quarter are available at
http://courses.washington.edu/mebi590/schedule.htm

Podcasts from previous quarters are available at
http://courses.washington.edu/mebi590/past.lecture.schedules.html