Fourth Biennial
Triangle Biophysics Symposium

Physics & Computation on Protein Structure

November 15-16, 2002
University of North Carolina at Chapel Hill • Hill Alumni Center

FRIDAY, NOVEMBER 15

9:00 - Welcome & Session I

STRUCTURE PREDICTION

• Computational Structural Biology: from Protein Evolution to Topological Classifiers
  Michael Levitt (Stanford, Computational Structural Biology)

• Prediction of Molecular Crystal Structures
  Robert Gdanitz (NC A&T, Physics)

• Computer-Based Design of Novel Protein Structures and Sequences
  Brian Kuhlman (UNC Chapel Hill, Biochemistry & Biophysics)

• Nonlinear Potential Derived from Alpha Shape and Chain Growth by Sequential Importance Sampling
  Jie Liang (U Illinois Chicago, Bioengineering)

12:15 - Lunch & Posters

2:15 - Session II

EXPLORING CONFORMATIONAL SPACES

• Identifying Motifs and Molegos in Protein Families and Superfamilies
  Werner Braun (UTMB Galveston, Human Biochemistry & Genetics)

• Shape Matching Algorithms for Proteins and Consensus Shapes of Protein Families
  Klara Kedem (Ben Gurion, Computer Science)

• Probabilistic Roadmaps: A Tool for Computing Ensemble Properties of Molecular Motions
  Jean-Claude Latombe (Stanford, Computer Science)

• Does Packing of Proteins Obey a Boltzmann Distribution, and What Does That Mean?
  Jan Hermans (UNC Chapel Hill, Biochemistry & Biophysics)

SATURDAY, NOVEMBER 16

9:00 - Session III

MODELING AND EXPERIMENTS

• Single Molecule Fluorescence Studies of Protein Folding
  William Eaton (NIH, Chemical Physics)

• Reaction Path of Protein Prenyltransferases at Atomic Resolution
  Lorena Beese (Duke, Biochemistry)

• Modeling Protein Flexibility in Molecular Recognition
  Leslie Kuhn (Michigan State, Biochemistry & Molecular Biology)

• Dissections of Protein Flexibility from Experimental and Theoretical Methods
  Andrew Lee (UNC Chapel Hill; Pharmacy)

12:05 - Lunch & Posters

2:00 - Session IV

SIMULATION FOR UNDERSTANDING

• Computer Simulation of Lipid Self-Assembly: from Micelles to Vesicles
  Siewert-Jan Marrink (Groningen, Biochemistry)

• Understanding the Origin of Amyloidosis from Molecular Dynamics Simulations
  Nikolay Dokholyan (UNC Chapel Hill, Biochemistry & Biophysics)

• Simulation of Chemical Reactions in Enzyme with a DFT QM/MM Free Energy Method
  Weitao Yang (Duke, Chemistry)

• What Proteins Don’t Do
  David and Jane Richardson (Duke, Biochemistry)

For More Info
Please visit the web site or contact Lisa Phillippie of the UNC Program in Molecular and Cellular Biophysics at 919-843-9737 or ldh@med.unc.edu.

Location
All events and the Carolina Inn hotel are located on the campus of the University of North Carolina, Chapel Hill, which is served by the Raleigh-Durham International Airport (RDU).

Mixers
Meet your colleagues at mixers on Thursday evening (Sitterson Hall lobby) and Friday evening (Hill Alumni Center) from 5:30 to 7:30.

Registration
Fee is $100. Student fee is $25. The fee covers the mixers, and coffee breaks and lunches on Friday and Saturday. The registration form is available on the TBS 2002 web site. Registration deadline is November 1.

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