

The TCBG and NIH Present: Hands-on Course in Computational Biology



Boston, MA & The Colonnade Hotel



The Program

Hands-on Course in Computational Biology



Prof. Klaus Schulten



Dr. Emad Tajkhorshid

Location: Braemore/Kenmore Room
Boston Ballroom (Tue, Dec. 7 only)

Handouts: Hands-on Sessions
Unix Primer
Mac Primer



Sun, 12/5: *Introduction to Protein Structure and Dynamics*



Braemore/Kenmore Room

09:00-09:30 Opening Remarks

09:30-10:40 Molecular Graphics Perspective of Protein Structure & Function

Break

11:00-11:50 Molecular Dynamics Method

11:50-12:00 Daily Q & A

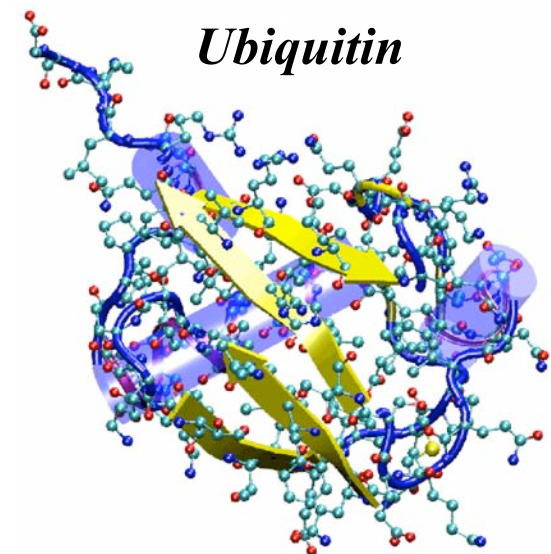
Lunch

14:00-14:45 Overview of Hands-on Sessions

15:00-15:30 Molecular Graphics Tutorial

Break

15:45-18:00 Molecular Graphics Tutorial /
Molecular Dynamics Tutorial



Mon, 12/6: *Introduction to Bioinformatics*



Braemore/Kenmore Room

09:00-10:00 Intro to Bioinformatics: Sequence, Structure, and Alignment

10:00-10:40 Evolutionary Concepts in Bioinformatics

Break

11:00-11:50 Application of Bioinformatics 1, 2

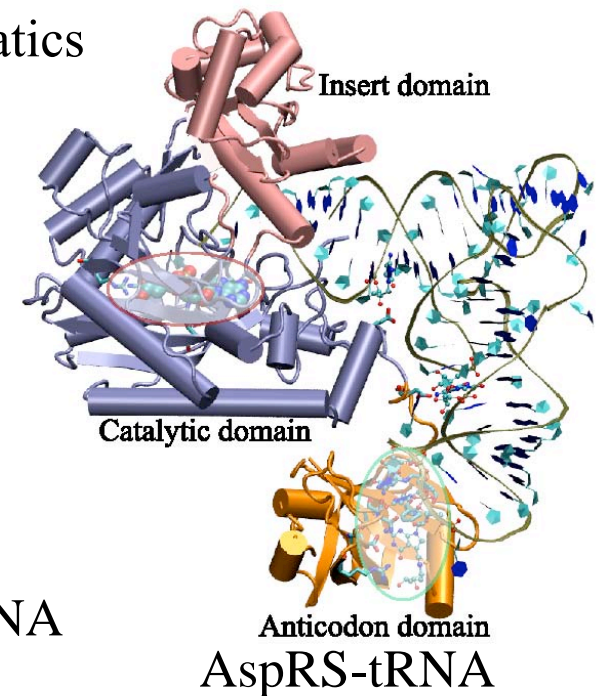
11:50-12:00 Daily Q & A

Lunch

14:00-16:00 Bioinformatics Study of Aquaporins

Break

Time permitting: Bioinformatics Study of Aspartyl-tRNA synthetase



Tue, 12/7: *Statistical Mechanics of Proteins*



Boston Ballroom

09:00-10:00 Equilibrium Properties of Proteins

10:00-10:40 Nonequilibrium Properties of Proteins

Break

11:00-11:50 Simulated Cooling of Proteins

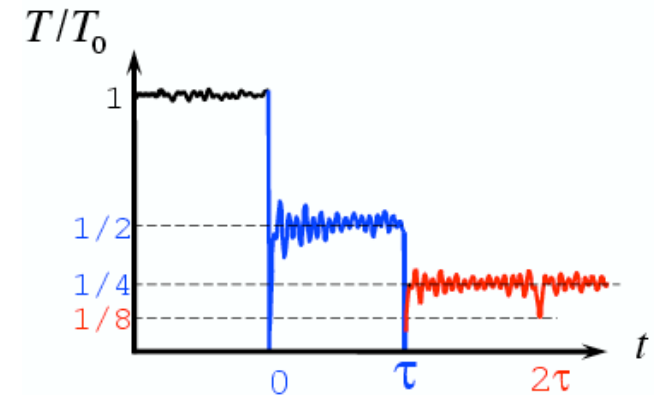
11:50-12:00 Daily Q & A

Lunch

14:00-15:30 Molecular Dynamics Tutorial

Break

15:45-18:00 Molecular Dynamics Tutorial (continued)



Wed, 12/8: *Parameters for Classical Force Fields*



Braemore/Kenmore Room

09:00-10:00 Introduction and Examples

10:00-10:40 Force Field Parameterization

Break

11:00-11:50 Applications

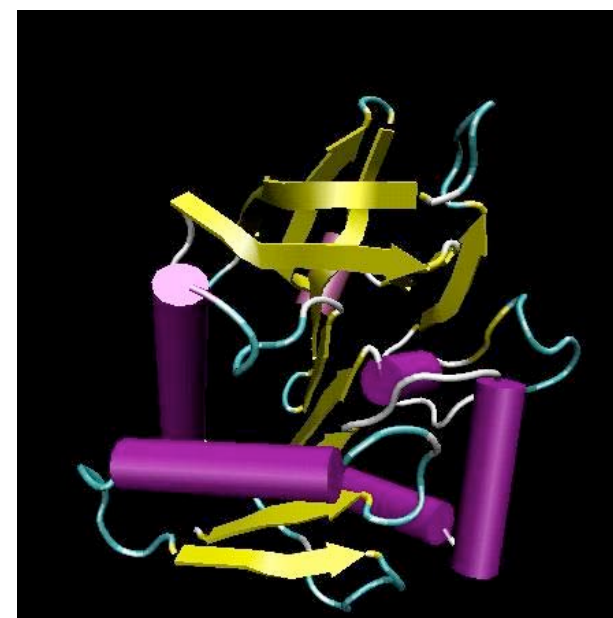
11:50-12:00 Daily Q&A

Lunch

14:00-15:30 Parameterizing a Novel Residue

Break

15:45-18:00 Topology File Tutorial

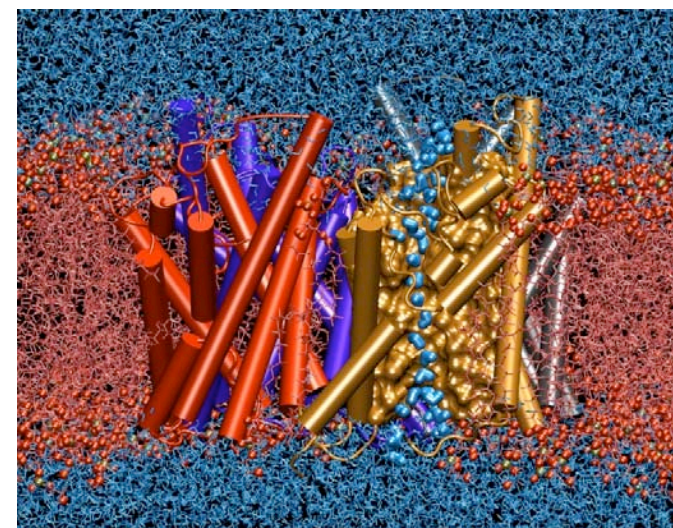


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Thu, 12/9: *Simulating Membrane Channels*



Water Permeation through Aquaporin



Braemore/Kenmore Room

09:00-10:00 Introduction and Examples

10:00-10:40 Transport in Aquaporins

Break

11:00-11:50 Nanotubes

11:50-12:00 Daily Q&A

Lunch

14:00-15:00 Nanotubes

15:00-15:30 Molecular Dynamics Tutorial (continued)

Break

15:45-18:00 Molecular Dynamics Tutorial (continued)

Acknowledgements

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Marcos Sotomayor



J.C. Gumbart



Patrick O'Donoghue

**Tutorials & Laptop
Preparation**



B. Dhaliwal



M. Bach



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