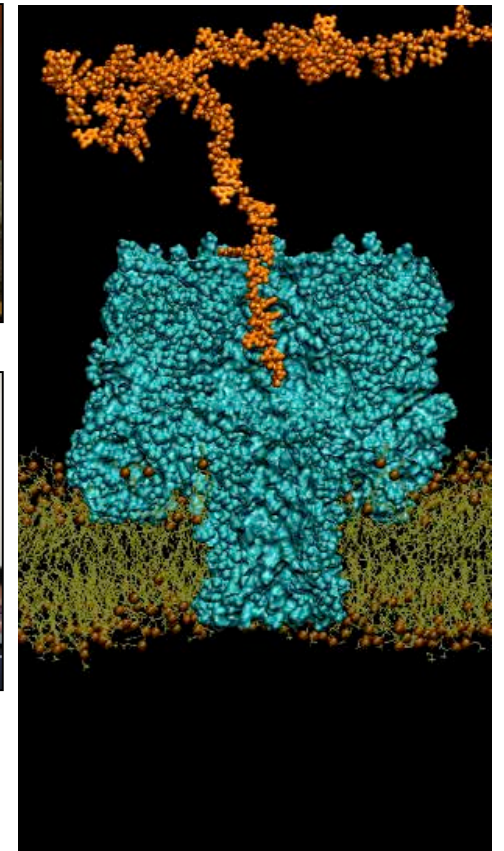
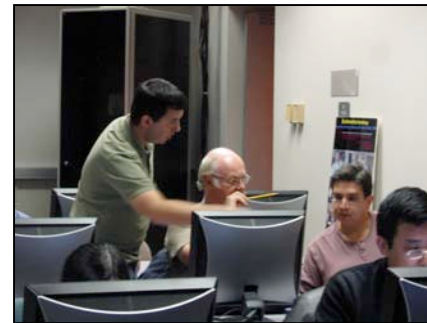


The TCBG & the Max Planck Institute Present: Hands-on Course in Computational Biology



Frankfurt, Germany



The Program

Hands-on Course in Computational Biology



Prof. Klaus Schulten



Prof. Zan Luthey-Schulten



Dr. Emad Tajkhorshid

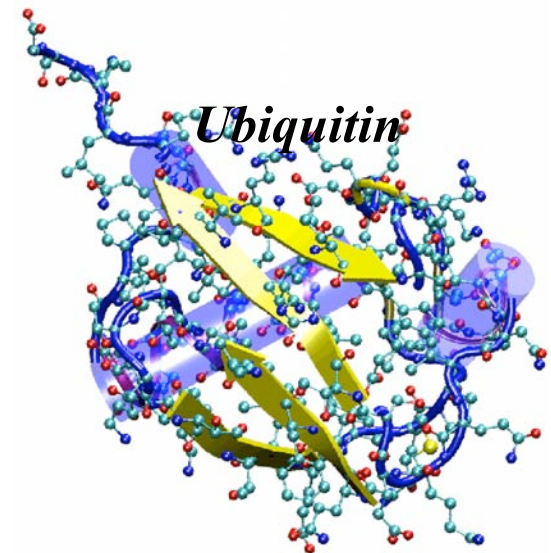
Max Planck Institute for Biophysics



Mon, 3/20: *Introduction to Protein Structure and Dynamics*



09:00-09:30	Opening Remarks
09:30-10:40	Molecular Graphics Perspective of Protein Structure & Function
<i>Break</i>	
11:00-11:50	Molecular Dynamics Method
11:50-12:00	Daily Q & A
<i>Lunch</i>	
14:00-14:45	Overview of Hands-on Sessions
15:00-15:30	Molecular Graphics Tutorial
<i>Break</i>	
15:45-18:00	Molecular Graphics Tutorial



Tue, 3/21: *Statistical Mechanics of Proteins*



09:00-10:00 Molecular Dynamics with NAMD

10:00-10:40 Equilibrium Properties of Proteins

Break

11:00-11:50 Nonequilibrium Properties of Proteins

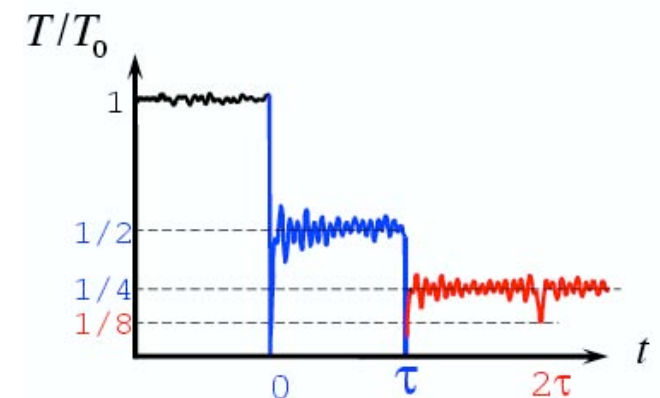
11:50-12:00 Daily Q & A
Group photo

Lunch

19:00-20:30 Molecular Dynamics Tutorial

Break

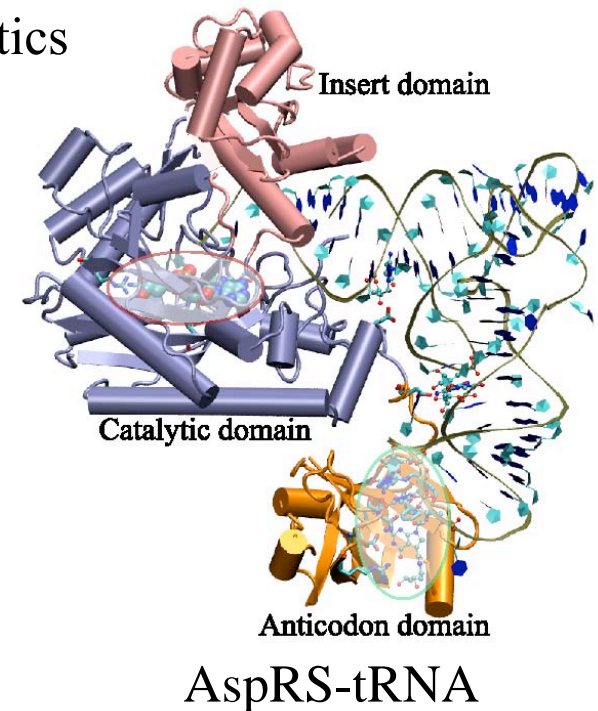
20:45-23:00 Molecular Dynamics Tutorial (continued)



Wed, 3/22: *Introduction to Bioinformatics*



09:00-10:00	Intro to Bioinformatics: Sequence, Structure, and Alignment
10:00-10:40	Evolutionary Concepts in Bioinformatics
<i>Break</i>	
11:00-11:50	Application of Bioinformatics
11:50-12:00	Daily Q & A
<i>Lunch</i>	
14:00-16:00	Evolution of Protein Structure – Aspartyl tRNA Synthetase
<i>Break</i>	
16:15-18:00	Evolution of Protein Structure – Aspartyl tRNA Synthetase continued



Thu, 3/23: *Simulating Membrane Channels*



Water Permeation through Aquaporin

09:00-10:00 Introduction and Examples

10:00-10:40 Transport in Aquaporins

Break

11:00-11:50 Nanotubes

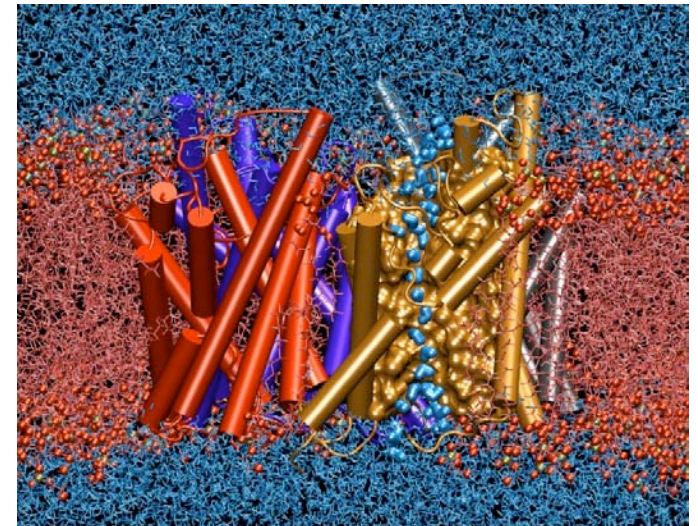
11:50-12:00 Daily Q&A

Lunch

14:00-15:30 Nanotubes/IMD

Break

15:45-18:00 Deca-alanine/Open tutorial work time



Acknowledgements

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J.C. Gumbart

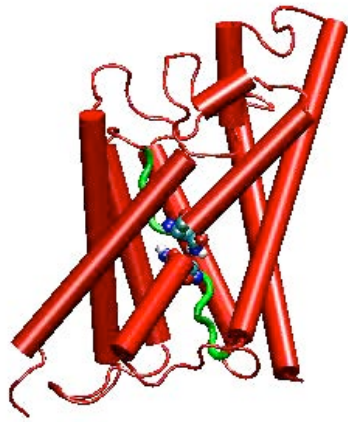


Elijah Roberts

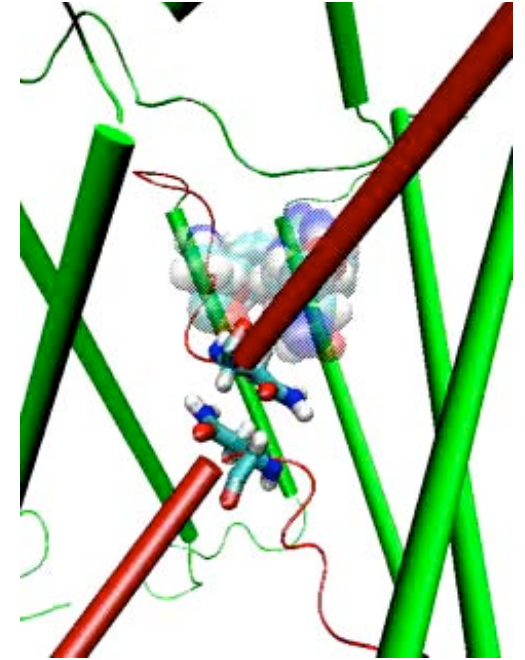


Yi Wang

and many members of the Klaus and Zan Schulten groups



General



- **The course is a volunteer effort**
 - **The main focus are the hands-on sessions**
 - **The aim is to get you to do computational biology**
 - **The lecturers / teaching assistants provide tutorials for you**
 - **The optimal course is that you help each other**
-
- **Please give us feedback to improve lectures and tutorials**

