

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



Beckman Institute



The Program

Hands-on Course in Computational Biology



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Location: 5269 Beckman Institute

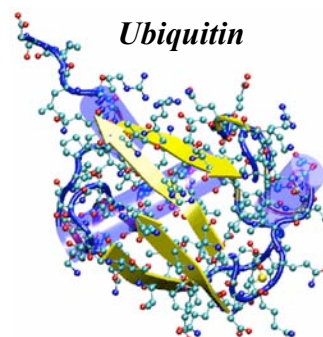
Handouts: Hands-on Sessions
Unix Primer
Mac Primer



Mon, 11/8: *Introduction to Protein Structure and Dynamics*



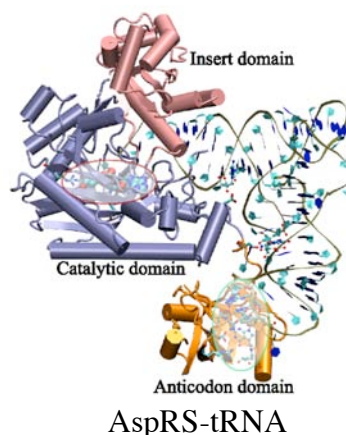
09:15-09:40	Opening Remarks
09:45-10:40	Molecular Graphics Perspective of Protein Structure & Function
<i>Break</i>	
10:50-11:50	Molecular Dynamics Method
11:50-12:00	Daily Q & A
<i>Lunch</i>	
14:00-14:40	Overview of Hands-on Sessions
14:45-18:00	Molecular Graphics Tutorial (R. Braun, M. Gao)



Tue, 11/9: *Introduction to Bioinformatics*



09:00-10:00	Sequence Structure and Alignment
10:00-10:40	Evolution of Protein Structure
<i>Break</i>	
11:00-11:50	The Biology and Bioinformatics of tRNA Synthetase and Aquaporins
11:50-12:00	Daily Q & A
<i>Lunch</i>	
14:00-18:00	Evolution of Protein Structure: tRNA Synthetases
Time permitting:	Bioinformatics of Aquaporins (P. O'Donoghue, J. Yu)



Wed, 11/10: *Statistical Mechanics of Proteins*



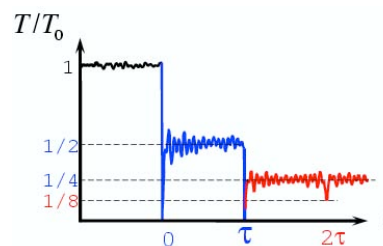
09:00-10:00 Equilibrium Properties of Proteins
 10:00-10:40 Nonequilibrium Properties of Proteins

Break

11:00-11:50 Simulated Cooling of Proteins
 11:50-12:00 Daily Q & A

Lunch

14:00-18:00 Molecular Dynamics Tutorial
 Deca-alanine Tutorial
 (M. Dittrich, T. Isgro)



Thu, 11/11: *Parameters for Classical Force Fields*



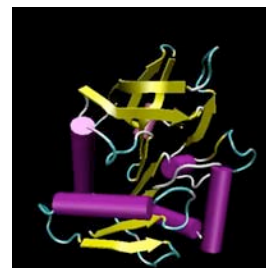
09:00-10:00 Introduction and Examples
 10:00-10:40 Introduction to Classical Force Fields

Break

11:00-11:50 Methods of Parameterization
 11:50-12:00 Daily Q&A

Lunch

14:00-15:30 System set-up of HisH with the Molecular Modeling package
 MOE
 15:30-18:00 Semiempirical Parameter Generation with Spartan
 (F. Khalili-Araghi, C. Kanchanawarin)



HisH

Fri, 11/12: *Simulating Membrane Channels*



09:00-10:00 Introduction and Examples

10:00-10:40 Transport in Aquaporins

Break

11:00-11:50 Nanotubes

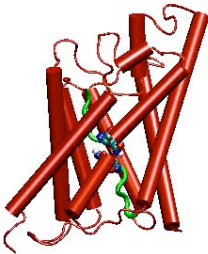
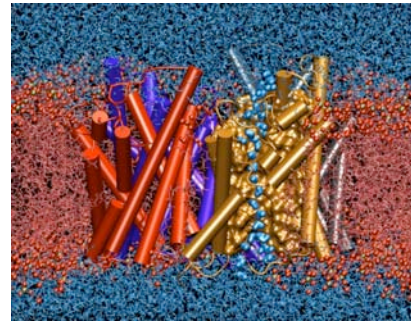
11:50-12:00 Daily Q&A

Lunch

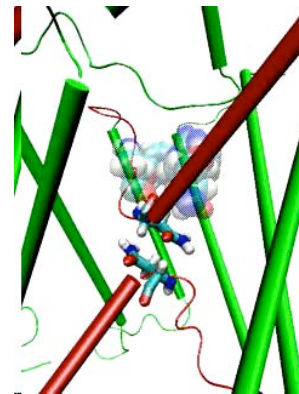
14:00-15:00 Bioinformatics of Aquaporins

15:00-18:00 Nanotubes
(J. Cohen, D. Lu)

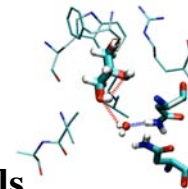
Water Permeation through Aquaporin



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
- Model your own system
- Please give us feedback to improve lectures and tutorials
- Please give us feedback to encourage future courses



Acknowledgements

A s s i s t a n t s



R. Braun



M. Gao



J. Yu



R. Amaro



M. Dittrich



T. Isgro



J. Cohen



C. Kanchanwarin



F. Khalili



D. Lu

Tutorials & Laptop Preparation



B. Dhaliwal



M. Bach



E. Villa