

Yuan (John) Yao

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EDUCATION

Stony Brook University, Stony Brook, NY

Dec. 2014

Ph.D. Applied Mathematics & Statistics (Computational Biology)

Shandong University, Jinan, China.

June 2010

B.S. School of Life Science (Microbiology)

SKILLS

Computational Skills:

- Programming: C/C++, Python, FORTRAN, B Shell script.
- Proficiency in Matlab and R.
- Experienced Linux OS and super computer cluster usage.
- Website design: HTML, CSS, JavaScript, jQuery, mySQL.
- Bio-molecular toolbox: Gromacs, Amber, NAMD, VMD, Chimera, AutoDock, GAMESS.
- Structural molecular modeling, Network modeling, Bioinformatics (Bioconductor).

Biological Experiments:

- Basic Microbiology, Cytology and Physiology experimental skills.
- Basic Molecular cloning, Chromatography and Electrophoresis.
- Basic MALDI-TOF mass spectrometry experience.
- Basic Structural NMR.

RESEARCH EXPERIENCE

Research Assistant, Dr. Jin Wang's group, Stony Brook University, NY

Aug. 2010 - Sept. 2015

- Discovered new binding-folding mechanism of Lambda Cro repressor.
- Built all-atom structure-based model for regulatory protein dimers.
- Performed replica exchange molecular dynamics (REMD) and weighted histogram analysis (WHAM).
- Built and visualized multi-dimensional free energy landscapes.
- Calculated activation barrier in enzymatic reaction with QM/MM method and umbrella sampling.

Side projects:

- Discovered epigenetic patterns of differentially methylated regions (DMRs) in Arabidopsis under high CO₂ pressure (with Dr. Alison Liu).
- Modeled binding poses of peptide inhibitor/activator of RNA polymerase (with Dr. Paul Freimuth).
- Statistically studied codon pair bias along evolution (a class project).
- Practiced BioNetGen in Rule-based modeling of biochemical systems (a class project).

Senior Year Internship, Dr. Niu Huang's computational chemistry laboratory,
National Institute of Biological Sciences (NIBS), Beijing

July 2009 - Feb. 2010

- Searched and collected data from PDB database for human disease related targets.
- Explored several biomedical databases (KEGG, DrugBank, PubChem, BioSystems).
- Experienced the environment of hierarchical virtual screening for drug discovery.

Undergraduate Research Assistant, Dr. Lushan Wang's group,
National Key Laboratory of Microbiology, Jinan, China

July 2008 - Jun. 2010

- Built free energy profile of Cellobiohydrolase I (CBHI) translocation on cellulose fiber, using steered molecular dynamics (SMD).
- Applied polyacrylamide gel electrophoresis (PAGE) to separate enzyme components in the fermentation of a filamentous fungus.

TEACHING EXPERIENCE

Instructor, Applied Calculus I (Enrolled: 119 undergraduates)

Aug. 2013- Dec. 2013

- Full semester lecturing: two 80 minutes lectures per week.
- Designed syllabus, supervised three TAs, created homework and examinations.

PUBLICATIONS

J. Yao and J. Wang. Neither Two-State nor Three-State: Dimerization of Lambda Cro Repressor. **J. Phys. Chem. Lett.**, 2015, 6, 2022–2026. (2015). [PDF](#)

John Yao and Jin Wang. Diverse protein dimerization mechanisms study with all-atom structure based model (pre-submission).

ACTIVITIES AND HONORS

- Founder and 1st President of an interdisciplinary graduate student club
- XCHANGE COOP (<http://www.xchangepcoop.org/>). May-Dec. 2014
- Organized and instructed Matlab plotting mini-workshop (80 minutes, 48 attendants). Oct. 31th, 2014
- Chief marketing person for a student startup group Lunchea.com. Aug. 2014 -Feb.2015
- Voluntary tennis coach for graduate students (weekly 2-hour lessons, 10 students). June 6-July 25, 2015

RELEVANT CLASSES

Algorithms in Bioinformatics	A
Numerical Methods and Algorithms in Computational Biology	A
Introduction to Systems Biology	A
Principles in Parallel Computing	A

HOBBIES

Ballroom dance, tennis, cycling, swimming; Handcrafting.

Webpage with YouTube channel: <http://xchangepcoop.org/people/john.html>