YANG SHEN

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Research Interests

- Modeling, simulation, and control of biomolecular networks, including drug design, protein docking, protein engineering, systems and synthetic biology, and bioinformatics.

Education and Training

- **Massachusetts Institute of Technology** — Cambridge, MA
  Postdoctoral Associate — 09/2008 – 12/2011
- **Boston University** — Boston, MA
  Postdoctoral Researcher — 09/2007 – 08/2008
  Ph.D. in Systems Engineering — 01/2008 (completed: 08/2007)
- **University of Science and Technology of China** — Hefei, China
  Bachelor of Engineering — 06/2002

Professional Experience

- **Texas A&M University** — College Station, TX
  Department of Electrical and Computer Engineering
  TEES–AgriLife Center for Bioinformatics and Genomic Systems Engineering
  Assistant Professor — 01/2015 – present
- **Toyota Technological Institute at Chicago** — Chicago, IL
  Research Assistant Professor — 01/2012 – 12/2014
- **Massachusetts Institute of Technology** — Cambridge, MA
  Departments of Biological Engineering and Electrical Engineering & Computer Science
  Computer Science and Artificial Intelligence Laboratory (CSAIL)
  Research Affiliate — 01/2012 – present
  Visiting Assistant Professor — 06/2012 – 07/2012

Honors and Awards

- My team ranked the 4th among 29 groups for performances predicting oligomeric protein structures in the 30th round of *CAPRI* (Critical Assessment of PRedicted Interactions), a community-wide experiment on comparative evaluation of protein docking methods. 12/2014

- "Dimension Reduction and Optimization Methods for Flexible Refinement of Protein Docking", *Principal Investigator*, $174,987, National Science Foundation.   10/2013 – 09/2015

- Director's Discretionary Award (sponsored by DOE), 3M CPU hours (IBM Blue Gene), Argonne Leadership Computing Facility, Argonne National Laboratory.   2012 – 2013

- My team tied at No. 5 among 64 participants in the 5th *CAPRI* Evaulation (2010–12). Invited talk at the *5th CAPRI Evaluation Meeting* (Utrecht, The Netherlands).　　04/2013

- Our team (led by Dr. Vajda) ranked No. 1 among 54 participants from 10 countries at the *4th CAPRI Evaluation Meeting* (Barcelona, Spain).　　12/2009
  Developed and applied a docking method *SDU* that refined initial models to medium- or high-quality predictions for 5 of 7 targets where we succeeded.

- First Prize, *3rd CAPRI Evaluation Meeting* (Toronto, Canada).　　04/2007

- CISE First Prize, Boston University Science and Engineering Day Symposium.　　03/2005

- Graduate Teaching Fellowship, Boston University.　　2002

- Guanghua Scholarship, USTC.　　2001

Teaching Experience

- **TAMU**
  - ECEN 303 *Random Signals and Systems*　　Spring 2015

- **TTIC**
  - Lecturer for *Introduction to Machine Learning* (3 lectures). Toyota Technological Institute, Nagoya, Japan.　　05/2014
  - Guest lecturer for *Intro. to Bioinformatics & Computational Biology* (2 lectures).　03/2012

- **MIT, Department of Biological Engineering**
  Co-advised two Ph.D. students in rotation projects.　　10/2009 – 01/2010, 12/2010 – 02/2011

- **Boston University, Division of Systems Engineering**
  - Co-advised two graduate students.　　04/2007 – 08/2007, 10/2007 – 08/2008
  - Teaching assistant for *Numerical Methods in Biomedical Engineering (Module on Optimization in Molecular Docking)*.　　Fall 2006
  - Guest lecturer for *Structural Bioinformatics* (3 lectures).　　Fall 2005
  - Teaching assistant for *Optimization Theory and Methods*.　　Fall 2004
  - Graduate Teaching Fellow for *Engineering Computation in C++*.　　2002 – 2003

Professional Services

- Associate Editor, EURASIP Journal on Bioinformatics and Systems Biology.　　2015–

- Member, Proceedings Committee (Area: Protein Structure and Function), *Annual International Conference on Intelligent Systems in Molecular Biology* (ISMB).　2014, 2015

- Member, Abstract Review Committee, *23rd Annual Symposium of the Protein Society*. 2009

- Reviewer for *Proteins*, *Journal of Proteomics & Bioinformatics*, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, *Protein Engineering Design & Selection*, *Journal of Chemical Theory and Computation*, *PLoS ONE*, *ISMB*, *RECOMB* and so on.

- Panelist for the National Science Foundation.

- Ad hoc reviewer for the National Science Foundation.

- Member of *American Chemical Society*, *Institute of Electrical and Electronics Engineers*, and *International Society for Computational Biology*.

Book Chapter

- D Beglov, R Brenke, G-Y Chuang, D Hall, M Landon, CH Ngan, **Y Shen**, S Thiel, B Zerbe, D Kozakov, and S Vajda, "Identification of Druggable Hot Spots on Proteins and in Protein Protein Interfaces", in *Computational Protein-Protein Interactions* (Ed. Ruth Nussinov and Gideon Schreiber), CRC Press, June 2009, pages 253–280.

Journal Articles

- **Y Shen**, ML Radhakrishnan, and B Tidor (2015) "Molecular Mechanisms and Design Principles for Promiscuous Inhibitors to Avoid Drug Resistance: Lessons Learned from HIV-1 Protease Inhibition", *Proteins: Structure, Function and Bioinformatics*, 83(2), 351–372.

- MF Lensink and 57 others including **Y Shen** (2014) "Blind Prediction of Interfacial Water Positions in CAPRI", *Proteins: Structure, Function and Bioinformatics* 82(4), 620–632.

- W Toy, **Y Shen**, H Won, B Green, RA Sakr, M Will, Z Li, K Gala, S Fanning, TA King, C Hudis, D Chen, T Taran, G Hortobagyi, GL Greene, M Berger, J Baselga, and S Chandarlapaty (2013) "*ESR1* Ligand-Binding Domain Mutations in Hormone-Resistant Breast Cancer", *Nature Genetics* 45(12), 1439–1445.

- **Y Shen** (2013) "Improved Flexible Refinement of Protein Docking in CAPRI Rounds 22–27", *Proteins: Structure, Function and Bioinformatics* 81(12), 2129–2136.

- **Y Shen**, MD Altman, A Ali, MNL Nalam, H Cao, TM Rana, CA Schiffer, and B Tidor (2013) "Testing the Substrate-Envelope Hypothesis with Designed Pairs of Compounds", *ACS Chemical Biology* 8(11), 2433–2441.

- MD Balbas, MJ Evans, DJ Hosfield, J Wongvipat, V Arora, PA Watson, Y Chen, GL Greene, **Y Shen***, and CL Sawyers* (2013) "Overcoming Mutation-Based Resistance to Antiandrogens with Rational Drug Design", *eLife* 2, e00499. (* Co-corresponding authors)

- **Y Shen**, MK Gilson, and B Tidor (2012) "Charge Optimization Theory for Induced-Fit Ligands", *Journal of Chemical Theory and Computation* 8(11), 4580–4592.

- D Kozakov, DR Hall, D Beglov, R Brenke, SR Comeau, **Y Shen**, K Li, J Zheng, P Vakili, ICh Paschalidis, and S Vajda (2010) "Achieving Reliability and High Accuracy in Automated Protein Docking: ClusPro, PIPER, SDU, and stability analysis in CAPRI rounds 13–19", *Proteins: Structure, Function and Bioinformatics* 78(15), 3124–3130.

- **Y Shen**, ICh Paschalidis, P Vakili, and S Vajda (2008)"Protein Docking by the Underestimation of Free Energy Funnels in the Space of Encounter Complexes", *PLoS Computational Biology* 4(10), e1000191.

- **Y Shen**, R Brenke, D Kozakov, SR Comeau, D Beglov, and S Vajda (2007) "Docking with PIPER and Refinement with SDU in Rounds 6–11 of CAPRI", *Proteins: Structure, Function and Bioinformatics* 69(4), 734–742.

- SR Comeau, D Kozakov, R Brenke, **Y Shen**, D Beglov, and S Vajda (2007) "ClusPro: Performance in CAPRI Rounds 6–11 and the New Server", *Proteins: Structure, Function and Bioinformatics* 69(4), 781–785.

- ICh Paschalidis, **Y Shen**, P Vakili, and S Vajda (2007) "SDU: A Semi-Definite Programming-Based Underestimation Method for Stochastic Global Optimization in Protein Docking", *IEEE Transactions on Automatic Control* 52(4), 664–676.

Conference Papers

- **Y Shen**, P Vakili, S Vajda, and ICh Paschalidis (2007) "Optimizing Noisy Funnel-like Functions on the Euclidean Group with Applications to Protein Docking", *Proceedings of the 46th IEEE Conference on Decision and Control* (CDC'07), 4545–4550, Dec. 12-14, 2007, New Orleans, Louisiana.

- ICh Paschalidis, **Y Shen**, P Vakili, and S Vajda (2006) "Protein–Protein Docking with Reduced Potentials by Exploiting Multi-Dimensional Energy Funnels", *Proceedings of the 28th IEEE International Conference of the Engineering in Medicine and Biology Society* (EMBC'06), 5330–5333, Aug. 2006, New York City, New York.

- ICh Paschalidis, **Y Shen**, P Vakili, and S Vajda (2005) "Semi-Definite Programming-Based Underestimation Method for Global Optimization in Molecular Docking", *Proceedings of the 44th IEEE Conference on Decision and Control* (CDC'05), 3675–3680, Dec. 2005, Seville, Spain.

Patent

- "Modulators of resistant androgen receptor" (with C. L. Sawyers et al.), U.S. patent, filed in Oct. 2012.

Selected Talks

(from 29 refereed conference abstracts)

1. "On Conformational Changes Associated with Protein-Protein Interactions: Normal Mode Analysis for Encounter Complexes" (with T. Oliwa), *2014 Protein Folding Conference*, **invited**, Jul. 16-19, 2014, Punta Cana, Dominican Republic.

2. "Improved flexible refinement of protein docking in CAPRI rounds 22–27", *5th CAPRI Evaluation Meeting* (CAPRI'13), **selected as regular lecture**, Apr. 17–19, 2013, Utrecht, The Netherlands.

3. "Designing and unraveling promiscuous inhibitors against drug-resistant target mutations" (with M Radhakrishnan and B Tidor), *245th ACS National Meeting* (ACS'13-S), **invited**, Apr. 7–11, 2013, New Orleans, Louisiana.

4. "Designing promiscuous inhibitors: Lessons learned from HIV-1 protease inhibition" (with M Radhakrishnan and B Tidor), *241st ACS National Meeting* (ACS'11-S), Mar. 27–31, 2011, Anaheim, California.

5. "Docking refinement by the underestimation of free energy funnels", **invited**, *4th Conference on Modeling of Protein Interactions* (MPI'07), Sept. 30–Oct. 2, 2007, Lawrence, Kansas.

6. "Structural similarity of binding sites in analogous enzymes" (with D Beglov, R Brenke, D Kozakov, and S Vajda), *234th ACS National Meeting* (ACS'07-F), Aug. 19–23, 2007, Boston, Massachusetts.