CURRICULUM VITAE

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PROFESSIONAL POSITIONS

09. 2012 – present	**Research Fellow** (Barry Grant's Lab), Dept Computational Medicine & Bioinformatics, University of Michigan
09. 2008 – 07. 2012	**Research Fellow** (Shoji Takada's Lab), Dept Biophysics, Grad School of Science, Kyoto University

EDUCATION

09. 2005 – 06. 2008	**Ph.D.,** Biomechanics and Medical Engineering, College of Engineering, Peking University (Advisors: Zhen-Su She & Huaiqiu Zhu. Title of dissertation: "A complex systems approach to study of protein structures")
09. 2002 – 06. 2005	Graduate student, Condensed Matter Physics, School of Physics, Peking University
09. 1998 – 06. 2002	**B.S.,** Applied Physics (Minored in Japanese), Dept Applied Physics, Hunan University

INTERNSHIP AND OTHER TRAINING

07. 2002 – 07. 2008	**RA,** Center for Theoretical Biology (Zhen-Su She's Lab), Peking University, Beijing, China
07. 2003	**Trainee,** School of Parallel Computing, Chinese Academy of Science, Beijing, China
10. 2004 – 12. 2004	**Internship,** Intel China Research Center, Beijing, China

TEACHING AND MENTORING

2003 (Fall)	**TA,** Statistical Physics, School of Physics, Peking University

GRANT APPLICATION

2015	**Co-I**, "G Protein Activation Mechanisms" (Proposal for allocation of simulation time on Anton at the Pittsburgh Supercomputing Center, Grant No. MCB150033P) **[Awarded]**

HORNORS AND AWARDS

2011	**The Best Talk,** "The 13th Annual Meeting of Chinese Life Science Association", Kyoto, Japan
2010	**The Best Poster,** "The 2nd Biosupercomputing Symposium", Tokyo, Japan
2008	**General Presentation Award,** "Bio-rad Forum of Graduate Students", Peking University, Beijing, China

2000	**General Scholarship,** Hunan University, Changsha, China
1999	**General Scholarship,** Hunan University, Changsha, China

AFFILLIATIONS AND SOCIAL SERVICES

Academic

2009 – present	Membership, Biophysical Society
2010 – 2012	Membership, Biophysical Society of Japan

Non-academic

2009 – 2012	General Secretary, Chinese Scholars Association in Kyoto
1999 – 2002	Student Committee, Dept. Applied Physics, Hunan University
1998 – 1999	President Assistant, Philately Society, Hunan University

SKILLS

OS	Linux, Windows, Mac OS X
Software	Amber, Gromacs, VMD, PyMol, AutoDock, Modeller, *etc*.
Programming	R, C, FORTRAN, BASH, Perl, Python, Tcl, *etc*.
Language	Mandarin Chinese (native), English (fluent), Japanese (daily communication)

REVIEWER OF JOURNALS

J Mol Graph Model, J Phys Chem, J Bioinform Comput Biol, PLoS ONE, Proteins

PUBLICATIONS

Peer Reviewed Journal Articles

1. Stender JD, Nwachukwu JC, Kastrata I, Kim Y, Strid T, Yakir M, Srinivasan S, Nowak J, Izard T, Erumbi R, Carlson KE, Katzenellenbogen JA, **Yao XQ**, Grant BJ, Leong HS, Lin CY, Frasor J, Nettles KW, Glass C. (2017) Structural and molecular mechanisms of cytokine-mediated endocrine resistance in human breast cancer cells. *Mol Cell* in press.
2. Nwachukwu JC, Srinivasan S, Bruno NE, Nowak J, Wright NJ, Minutolo F, Erumbi R, Izard T, **Yao XQ**, Grant BJ, Kojetin DJ, Elemento O, Katzenellenbogen JA, Nettles KW. (2016) Super-resolution structural analysis predicts environmental and synthetic estrogen activity. *Cell Chem Biol* in press.
3. Jariwala S, Skjærven L, **Yao XQ**, and Grant BJ. (2016) Investigating protein sequence-structure-dynamics relationships with Bio3D-web. *J Vis Exp* in press.
4. **Yao XQ**, Skjærven L, and Grant BJ. (2016) Rapid characterization of allosteric networks with ensemble normal mode analysis. *J Phys Chem B* 120:8276-88.
5. Skjærven L, Jariwala S, **Yao XQ**, and Grant BJ. (2016) Online interactive analysis of protein structure ensembles with Bio3D-web. *Bioinformatics* in press.
6. **Yao XQ**, Malik RU, Griggs NW, Skjaerven L, Traynor JR, Sivaramakrishnan S, and Grant BJ. (2016) Dynamic coupling and allosteric networks in the alpha subunit of heterotrimeric G proteins. *J Biol Chem* 291:4742-53.
7. Scarabelli G, Soppina V, **Yao XQ**, Atherton J, Moores C, Verhey K, and Grant BJ. (2015) Mapping the processivity determinants of the kinesin-3 motor domain. *Biophys J* 109:1537-40.
8. Skjaerven L, **Yao XQ**, Scarabelli G, and Grant BJ (2014) Integrating protein structural dynamics and evolutionary analysis with Bio3D. *BMC Bioinformatics* 15:399.

9. **Yao XQ** and Grant BJ. (2013) Domain-opening and dynamic coupling in the α-subunit of heterotrimeric G proteins. *Biophys J* 105:L08-10.
10. **Yao XQ**, Kimura N, Murakami S, and Takada S. (2013) Drug uptake pathways of multidrug transporter AcrB studied by molecular simulations and site-directed mutagenesis experiments. *J Am Chem Soc* 135:7474-85.
11. Kenzaki H, Koga N, Hori N, Kanada R, Li WF, Okazaki K, **Yao XQ,** and Takada S. (2011) CafeMol: a coarse-grained biomolecular simulator for simulating proteins at work. *J Chem Theory Comput* 7:1979-89.
12. †**Yao XQ**, Kenzaki H, Murakami S, and Takada S. (2010) Drug export and allosteric coupling in a multidrug transporter revealed by molecular simulations. *Nature Commun* 1**:**117.
13. Gao M, Zhu HQ, **Yao XQ**, and She ZS. (2010) Water dynamics clue to key residues in protein folding. *Biochem Biophys Res Comm* 392:95-9.
14. Gao M, **Yao XQ**, She ZS, Liu ZR, and Zhu HQ (2010) Intermediate structure and slow hydration water dynamics in protein folding process. *Acta Physico-chimica Sinica* 26:1998-2006.
15. Kang H, **Yao XQ**, She ZS, and Zhu HQ. (2009) Water-protein interplay reveals the specificity of alpha-lytic protease. *Biochem Biophys Res Comm* 385:165-9.
16. **Yao XQ** and She ZS. (2008) Key residue-dominated protein folding dynamics. *Biochem Biophys Res Comm* 373**:**64-8.
17. **Yao XQ**, Zhu HQ, and She ZS. (2008) A dynamic Bayesian network approach to protein secondary structure prediction. *BMC Bioinformatics* 9:49.

Talks

- "Dynamic coupling and activation mechanisms of heterotrimeric G proteins", (2016) *Cytoskeleton Seminar*, University of Michigan
- "Dynamic coupling and allosteric networks in the alpha subunit of heterotrimeric G proteins", (2015) *Sigtrans Seminar*, University of Michigan
- "G protein allosteric networks from molecular dynamics and normal mode analysis", (2014) *Sigtrans Seminar*, University of Michigan
- "Probing the activation mechanism of heterotrimeric G proteins with multiscale molecular simulations", (2014) *Tools and Technology Seminar*, University of Michigan
- "Nucleotide-dependent Transitions of the alpha-subunit of heterotrimeric G proteins probed with computational methods", (2013*) Sigtrans Seminar*, University of Michigan
- "Drug translocation and allosteric coupling in a multidrug transporter studied by molecular simulations", (2011) ***The 17th International Biophysics Congress (IUPAC),*** Beijing, China
- "Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulations", (2011) *The 13th Annual Meeting of Chinese Life Science Association*, Kyoto, Japan
- "The uptake and export of drugs in a multidrug transporter studied by coarse-grained simulations", (2011) ***The 49th Annual Meeting of the Biophysical Society of Japan****, Himeji*, Japan
- "Drug export and allosteric coupling in a multidrug transporter revealed by molecular simulations", (2011) *New Era of Biosimulations with Supercomputers*, Osaka, Japan

† Breaking scientific news in: *The Nikkei Business Daily* (Nov. 17, 2010), *The Nikkan Kogyo Shimbun* (Nov. 22, 2010), and *The Kyoto Shimbun* (Nov. 17, 2010).

- "Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation", (2010) ***The 47th Annual Meeting of the Biophysical Society of Japan***, Tokushima, Japan
- "Rotatory mechanism of AcrB transporter studied by coarse-grained simulation", (2009) *Workshop for Next-Generation Integrated Simulation of Living Matters on Molecular Scale*, Tokyo, Japan
- "Protein sequence, structure, and dynamics", (2007) *Institute for theoretical physics, Chinese Academy of Science*, Beijing, China

Posters

- **Yao XQ**, Malik RU, Griggs NW, Skjaerven L, Traynor JR, Sivaramakrishnan S, Grant BJ. Dynamic coupling and allosteric networks in the alpha subunit of heterotrimeric G proteins. (2016) *The 60th Annual Meeting of Biophysical Society*, LA.
- Skjaerven L, Jariwala S, Yao XQ, Ide J, Grant BJ. The Bio3D project: interactive tools for Structural Bioinformatics. (2016) *The 60th Annual Meeting of Biophysical Society*, LA.
- Skjaerven L, **Yao XQ**, Jariwala S, Grant BJ. Bio3D: interactive tools for structural bioinformatics. (2016) *The 60th Annual Meeting of Biophysical Society*, LA.
- Scarabelli G, Soppina V, **Yao XQ**, Atherton J, Moores CA, Verhey KJ, Grant BJ. Mapping the processivity determinants of the kinesin-3 motor domain. (2016) *The 60th Annual Meeting of Biophysical Society*, LA.
- Li H, **Yao XQ,** Grant BJ. Comparative structure dynamic analysis of G proteins. (2016) *The 60th Annual Meeting of Biophysical Society*, LA.
- **Yao XQ**, Skjaerven L, Grant BJ. Characterizing nucleotide dependent allostery in G-proteins with molecular dynamics and normal mode analysis. (2015) *Symposium on Computational Discovery in Complex Systems Biology*, University of Michigan.
- **Yao XQ,** Skjaerven L, and Grant BJ. G-protein allosteric networks from molecular dynamics and normal mode analysis (2015) *The 59th Annual Meeting of Biophysical Society*, Baltimore
- **Yao XQ**, Scarabelli G, Skjaerven L, Grant BJ. The Bio3D package: new interactive tools for Structural Bioinformatics. (2014) *The 58th Annual Meeting of Biophysical Society*, San Francisco
- **Yao XQ,** Jariwala S, and Grant BJ. Predicting HLA-specific drug hypersensitivity with molecular docking and molecular dynamics simulation. (2014) *The 58th Annual Meeting of Biophysical Society*, San Francisco
- **Yao XQ** and Grant BJ. Nucleotide-dependent transitions of the alpha subunit of heterotrimeric G-proteins probed with accelerated molecular dynamics simulations. (2013) *The 57th Annual Meeting of Biophysical Society*, Philadelphia
- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation: exploring the binding pathways of drugs. (2011) *The 55th Annual Meeting of Biophysical Society*, Baltimore
- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulations. (2010) *The 54th Annual Meeting of the Biophysical Society*, San Francisco
- Kenzaki H, Koga N, Fujiwara S, Hori N, Kanada R, Okazaki K, **Yao XQ**, Li WF, Takada S. Biomolecular coarse-grained simulation program CafeMol. (2010) *The 54th Annual Meeting of the Biophysical Society*, San Francisco
- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of multidrug transporter studied by coarse-grained simulations. (2010) *The 48th Annual Meeting of the Biophysical Society of Japan*, Sendai, Japan

- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation. (2010) *The 2nd Biosupercomputing Symposium*, Tokyo, Japan
- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation. (2010) *The 4th International Symposium on Molecular Science of Fluctuations toward Biological Functions*, Shiga, Japan

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References are available upon request.