CURRICULUM VITAE

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APPOINTMENTS

05. 2017 – present	**Postdoctoral Research Associate** (The Hamelberg Lab), Dept Chemistry, Georgia State University
09. 2012 – 04. 2017	**Postdoctoral Research Fellow** (The Grant Lab), Dept Computational Medicine & Bioinformatics, the University of Michigan
09. 2008 – 07. 2012	**Postdoctoral Research Fellow** (The Takada 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

TRAINING

07. 2002 – 07. 2008	**RA,** Center for Theoretical Biology (The She 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
2013 (Summer)	**Co-Mentor,** Undergraduate Research Opportunity Program (UROP), the University of Michigan

GRANTS

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

HONORS 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

AFFILIATIONS AND 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
Software	Amber, Gromacs, AutoDock, Modeller, VMD, PyMol, *etc*.
Programming	R, C/C++, FORTRAN, Bash, Perl, Python, Tcl, *etc*.
Language	Mandarin Chinese (native), English (fluent), Japanese (daily communication)
Expertise	molecular dynamics, coarse-grained molecular modeling and simulation, normal mode analysis, free energy calculation (FEP, umbrella sampling, MM-GB/SA, LIE), homology modeling, molecular docking, PCA, HMM, Bayesian network, dynamic Bayesian network, neural network

REVIEWER

Journals:

Proteins, BMC Bioinformatics, PLoS ONE, J Mol Graph Model, J Phys Chem, J Bioinform Comput Biol, Comp Biol & Chem

Conferences:

2017's Scientific Computing Day, Atlanta

PUBLICATIONS

*Peer-reviewed Journal Articles (*Joint-First Authors)*

- Vu PJ*, **Yao XQ***, Momin M, and Hamelberg D. Unraveling allosteric mechanisms of enzymatic catalysis with an evolutionary analysis of residue-residue contact dynamical changes. *PNAS (under review)*
- **Yao XQ*,** Jariwala S*, and Grant BJ. *In silico* prediction of HLA-associated drug hypersensitivity. *In preparation*.

1. **Yao XQ***, Cato MC*, Labudde E, Beyett TS, Tesmer JJG, and Grant BJ. Navigating the conformational landscape of G protein-coupled receptor kinases during allosteric activation. *J Biol Chem*. (2017) 292:16032-16043. [link]
2. **Yao XQ**, Skjærven L, and Grant BJ. Rapid characterization of allosteric networks with ensemble normal mode analysis. *J Phys Chem B* (2016) 120:8276-8288. [link]
3. **Yao XQ***, Malik RU*, Griggs NW, Skjaerven L, Traynor JR, Sivaramakrishnan S, and Grant BJ. Dynamic coupling and allosteric networks in the alpha subunit of heterotrimeric G proteins. *J Biol Chem* (2016) 291:4742-4753. [link]
4. **Yao XQ** and Grant BJ. Domain-opening and dynamic coupling in the α-subunit of heterotrimeric G proteins. *Biophys J* (2013) 105:L08-L10. [link]
5. **Yao XQ**, Kimura N, Murakami S, and Takada S. Drug uptake pathways of multidrug transporter AcrB studied by molecular simulations and site-directed mutagenesis experiments. *J Am Chem Soc* (2013) 135:7474-7485. [link]

6. **Yao XQ**, Kenzaki H, Murakami S, and Takada S. Drug export and allosteric coupling in a multidrug transporter revealed by molecular simulations. *Nature Commun* (2010) 1**:**117. (The work was reported by public media: *Nikkei Business Daily*, *Nikkan Kogyo Shimbun*, and *Kyoto Shimbun*). [link]
7. **Yao XQ** and She ZS. Key residue-dominated protein folding dynamics. *Biochem Biophys Res Comm* (2008) 373**:**64-68. [link]
8. **Yao XQ**, Zhu HQ, and She ZS. A dynamic Bayesian network approach to protein secondary structure prediction. *BMC Bioinformatics* (2008) 9:49. [link]
- Li H, **Yao XQ**, and Grant BJ. Comparative structural dynamic analysis of GTPases. *To be submitted*.
9. Bouley R, Waldschmidt HV, Cato MC, Cannavo A, Song J, Cheung JY, **Yao XQ**, Koch WJ, Larsen SD, and Tesmer JJG. Structural determinants influencing the potency and selectivity of indazole-paroxetine hybrid G protein-coupled receptor kinase 2 inhibitors. *Mol Pharmacol* (2017), in press. https://doi.org/10.1124/mol.117.110130.
10. 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. Structural and molecular mechanisms of cytokine-mediated endocrine resistance in human breast cancer cells. *Mol Cell* (2017) 65:1122-1135.e5. [link]
11. Nwachukwu JC, Srinivasan S, Bruno NE, Nowak J, Wright NJ, Minutolo F, Rangarajan ES, Izard T, **Yao XQ**, Grant BJ, Kojetin DJ, Elemento O, Katzenellenbogen JA, Nettles KW. systems structural biology analysis of ligand effects on ERα predicts cellular response to environmental estrogens and anti-hormone therapies. *Cell Chem Biol* (2017) 24:35-45. [link]
12. Jariwala S, Skjærven L, **Yao XQ**, and Grant BJ. Investigating protein sequence-structure-dynamics relationships with Bio3D-web. *J Vis Exp* (2017) 125:e55640. [link]
13. Skjærven L, Jariwala S, **Yao XQ**, and Grant BJ. Online interactive analysis of protein structure ensembles with Bio3D-web. *Bioinformatics* (2016) 32:3510-3512. [link]
14. Scarabelli G, Soppina V, **Yao XQ**, Atherton J, Moores C, Verhey K, and Grant BJ. Mapping the processivity determinants of the kinesin-3 motor domain. *Biophys J* (2015) 109:1537-1540. [link]
15. Skjaerven L, **Yao XQ**, Scarabelli G, and Grant BJ. Integrating protein structural dynamics and evolutionary analysis with Bio3D. *BMC Bioinformatics* (2014) 15:399. [link]
16. Kenzaki H, Koga N, Hori N, Kanada R, Li WF, Okazaki K, **Yao XQ,** and Takada S. CafeMol: a coarse-grained biomolecular simulator for simulating proteins at work. *J Chem Theory Comput* (2011) 7:1979-1989. [link]
17. Gao M, Zhu HQ, **Yao XQ**, and She ZS. Water dynamics clue to key residues in protein folding. *Biochem Biophys Res Comm* (2010) 392:95-99. [link]
18. Gao M, **Yao XQ**, She ZS, Liu ZR, and Zhu HQ. Intermediate structure and slow hydration water dynamics in protein folding process. *Acta Physico-chimica Sinica* (2010) 26:1998-2006. [link]
19. Kang H, **Yao XQ**, She ZS, and Zhu HQ. Water-protein interplay reveals the specificity of alpha-lytic protease. *Biochem Biophys Res Comm* (2009) 385:165-169. [link]

Talks

- "Allosteric modulation of G protein-coupled receptor kinase (GRK) activation," *Sigtrans Seminar*, University of Michigan (2017)
- "Dynamic coupling and activation mechanisms of heterotrimeric G proteins," *Cytoskeleton Seminar*, University of Michigan (2016)
- "Dynamic coupling and allosteric networks in the alpha subunit of heterotrimeric G proteins," *Sigtrans Seminar*, University of Michigan (2015)
- "G protein allosteric networks from molecular dynamics and normal mode analysis," *Sigtrans Seminar*, University of Michigan (2014)
- "Probing the activation mechanism of heterotrimeric G proteins with multiscale molecular simulations," *Tools and Technology Seminar*, University of Michigan (2014)
- "Nucleotide-dependent Transitions of the alpha-subunit of heterotrimeric G proteins probed with computational methods," *Sigtrans Seminar*, University of Michigan (2013)

- "Drug translocation and allosteric coupling in a multidrug transporter studied by molecular simulations," ***The 17th International Biophysics Congress (IUPAC)*****,** Beijing, China (2011)
- "Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulations," *The 13th Annual Meeting of Chinese Life Science Association*, Kyoto, Japan (2011)
- "The uptake and export of drugs in a multidrug transporter studied by coarse-grained simulations," ***The 49th Annual Meeting of the Biophysical Society of Japan****, Himeji*, Japan (2011)
- "Drug export and allosteric coupling in a multidrug transporter revealed by molecular simulations," *New Era of Biosimulations with Supercomputers*, Osaka, Japan (2011)
- "Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation," ***The 47th Annual Meeting of the Biophysical Society of Japan***, Tokushima, Japan (2009)
- "Rotatory mechanism of AcrB transporter studied by coarse-grained simulation," *Workshop for Next-Generation Integrated Simulation of Living Matters on Molecular Scale*, Tokyo, Japan (2009)
- "Protein sequence, structure, and dynamics," *Institute for theoretical physics, Chinese Academy of Science*, Beijing, China (2007)

Posters

- **Yao XQ**, Jariwala S, Grant BJ. In silico prediction of HLA-associated drug hypersensitivity. *The 61st Annual Meeting of Biophysical Society*, New Orleans (2017)
- **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. *The 60th Annual Meeting of Biophysical Society*, LA (2016)
- Skjaerven L, Jariwala S, Yao XQ, Ide J, Grant BJ. The Bio3D project: interactive tools for Structural Bioinformatics. *The 60th Annual Meeting of Biophysical Society*, LA (2016)
- Skjaerven L, **Yao XQ**, Jariwala S, Grant BJ. Bio3D: interactive tools for structural bioinformatics. *The 60th Annual Meeting of Biophysical Society*, LA (2016)
- Scarabelli G, Soppina V, **Yao XQ**, Atherton J, Moores CA, Verhey KJ, Grant BJ. Mapping the processivity determinants of the kinesin-3 motor domain. *The 60th Annual Meeting of Biophysical Society*, LA (2016)
- Li H, **Yao XQ,** Grant BJ. Comparative structure dynamic analysis of G proteins. *The 60th Annual Meeting of Biophysical Society*, LA (2016)
- **Yao XQ**, Skjaerven L, Grant BJ. Characterizing nucleotide dependent allostery in G-proteins with molecular dynamics and normal mode analysis. *Symposium on Computational Discovery in Complex Systems Biology*, University of Michigan (2015)
- **Yao XQ,** Skjaerven L, and Grant BJ. G-protein allosteric networks from molecular dynamics and normal mode analysis. *The 59th Annual Meeting of Biophysical Society*, Baltimore (2015)
- **Yao XQ**, Scarabelli G, Skjaerven L, Grant BJ. The Bio3D package: new interactive tools for Structural Bioinformatics. *The 58th Annual Meeting of Biophysical Society*, San Francisco (2014)
- **Yao XQ,** Jariwala S, and Grant BJ. Predicting HLA-specific drug hypersensitivity with molecular docking and molecular dynamics simulation. *The 58th Annual Meeting of Biophysical Society*, San Francisco (2014)
- **Yao XQ** and Grant BJ. Nucleotide-dependent transitions of the alpha subunit of heterotrimeric G-proteins probed with accelerated molecular dynamics simulations. *The 57th Annual Meeting of Biophysical Society*, Philadelphia (2013)
- **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. *The 55th Annual Meeting of Biophysical Society*, Baltimore (2011)
- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulations. *The 54th Annual Meeting of the Biophysical Society*, San Francisco (2010)

- Kenzaki H, Koga N, Fujiwara S, Hori N, Kanada R, Okazaki K, **Yao XQ**, Li WF, Takada S. Biomolecular coarse-grained simulation program CafeMol. *The 54th Annual Meeting of the Biophysical Society*, San Francisco (2010)
- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of multidrug transporter studied by coarse-grained simulations. *The 48th Annual Meeting of the Biophysical Society of Japan*, Sendai, Japan (2010)
- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation. *The 2nd Biosupercomputing Symposium*, Tokyo, Japan (2010)
- **Yao XQ**, Kenzaki H, and Takada S. Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation. *The 4th International Symposium on Molecular Science of Fluctuations toward Biological Functions*, Shiga, Japan (2010)

References are available upon request.