

## CURRICULUM VITAE

### Xin-Qiu YAO, Ph.D.

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### PROFESSIONAL POSITIONS

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

### EDUCATION

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09. 2005 – 06. 2008	<b>Ph.D.</b> , Biomechanics and Medical Engineering, College of Engineering, Peking University (Advisors: Zhen-Su She & Huaqiu 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>B.S.</b> , Applied Physics (Minored in Japanese), Dept Applied Physics, Hunan University

### INTERNSHIP AND OTHER TRAINING

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07. 2002 – 07. 2008	<b>RA</b> , 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	<b>Internship</b> , Intel China Research Center, Beijing, China

### TEACHING AND MENTORING

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2003 (Fall)	<b>TA</b> , Statistical Physics, School of Physics, Peking University
2013 (Summer)	<b>Co-Mentor</b> , Undergraduate Research Opportunity Program (UROP), University of Michigan

### GRANT APPLICATION

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2015	<b>Co-I</b> , "G Protein Activation Mechanisms" (Proposal for allocation of simulation time on Anton at the Pittsburgh Supercomputing Center, Grant No. MCB150033P) [ <b>Awarded</b> ]
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### HONORS AND AWARDS

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2011	<b>The Best Talk</b> , "The 13th Annual Meeting of Chinese Life Science Association", Kyoto, Japan
2010	<b>The Best Poster</b> , "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 SOCIAL SERVICES

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### 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

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OS	Linux, Windows, Mac OS X
Software	Amber, Gromacs, AutoDock, Modeller, VMD, PyMol, <i>etc.</i>
Programming	R, C, FORTRAN, BASH, Perl, Python, Tcl, <i>etc.</i>
Language	Mandarin Chinese (native), English (fluent), Japanese (daily communication)
Expertise	MD, coarse-grained model, elastic network model, normal mode analysis, FEP, umbrella sampling, MM-GB (PB)/SA, WHAM, homology modeling, docking, PCA, HMM, Bayesian network, dynamic Bayesian network, neural network

## REVIEWER OF JOURNALS

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

## PUBLICATIONS

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### 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, Frasier J, Nettles KW, Glass C. (2017) Structural and molecular mechanisms of cytokine-mediated endocrine resistance in human breast cancer cells. *Mol Cell* 65:1122-1135.e5.
2. 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. (2017) Systems Structural Biology Analysis of Ligand Effects on ER $\alpha$  Predicts Cellular Response to Environmental Estrogens and Anti-hormone Therapies. *Cell Chem Biol* 24:35-45.
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* 32:3510-3512.
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. \*Joint first authors.
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  $\alpha$ -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. <sup>†</sup>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
- “Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation”, (2009) **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

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<sup>†</sup> The work was reported in public media: *Nikkei Business Daily* (Nov. 17, 2010), *Nikkan Kogyo Shimbun* (Nov. 22, 2010), and *Kyoto Shimbun* (Nov. 17, 2010).

- **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 60<sup>th</sup> 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 60<sup>th</sup> Annual Meeting of Biophysical Society*, LA.
- Skjaerven L, **Yao XQ**, Jariwala S, Grant BJ. Bio3D: interactive tools for structural bioinformatics. (2016) *The 60<sup>th</sup> 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 60<sup>th</sup> Annual Meeting of Biophysical Society*, LA.
- Li H, **Yao XQ**, Grant BJ. Comparative structure dynamic analysis of G proteins. (2016) *The 60<sup>th</sup> 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 59<sup>th</sup> 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 58<sup>th</sup> 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 58<sup>th</sup> 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 57<sup>th</sup> 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 55<sup>th</sup> 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 54<sup>th</sup> 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 54<sup>th</sup> 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 48<sup>th</sup> 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 2<sup>nd</sup> 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 4<sup>th</sup> International Symposium on Molecular Science of Fluctuations toward Biological Functions*, Shiga, Japan

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References are available upon request.