Xinqiu YAO, Ph.D.

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EXPERTISE: bioinformatics, computational chemistry, molecular dynamics, coarse-grained models, molecular modeling, docking, free energy calculation, machine learning, genome informatics

EDUCATION

2008 **Ph.D.** (Biomechanics and Medical Engineering), College of Engineering, Peking University. Title of dissertation: "*A Complex Systems Approach to Studies of Protein Structures.*"

2002 **B.Sc.** (Applied Physics), Dept Applied Physics, Hunan University

APPOINTMENTS AND RESEARCH EXPERIENCE

2017–present **Postdoctoral Associate** in Chemistry (Hamelberg lab), Georgia State University

- Developing new computational methods for understanding protein function and allosteric regulation.
- Elucidating mechanisms underlying human enzymes with MD.

2012–2017 **Postdoctoral Fellow** in Computational Medicine and Bioinformatics (Grant lab), University of Michigan

- A lead developer of Bio3D, an R package for biomolecular sequence, structure, dynamics, and evolution analysis. Also developed Bio3D-web, a web application for interactive online structural analysis.
- Developed a new ensemble correlation network analysis method for understanding protein allosteric regulation and applied it to elucidate the activation mechanisms in heterotrimeric G proteins.
- Developed a new ensemble normal mode analysis for exploring dynamical aspects from structural biological data.
- Identified the allosteric pathway during the activation of GPCR kinases.
- HLA-specific drug hypersensitivity characterization and prediction using molecular docking, MD, and binding free energy calculations.
- Activation and allosteric mechanisms in estrogen receptors.

2008–2012 **Postdoctoral Fellow** in Biophysics (Takada lab), Kyoto University

- Elucidated mechanisms underlying drug export in the multidrug transporter AcrB with coarse-grained molecular simulations.
- Developed CafeMol, a software package for coarse-grained biomolecular modeling and simulations.

2002–2008 **Research Assistant**, Center for Theoretical Biology (She & Zhu lab), Peking University

- Protein secondary structure prediction with dynamic Bayesian networks and neural networks.
- Investigated the folding mechanisms of the small protein Trp-cage with MD.
- Developed algorithms for prokaryotic gene identification.

2004 **Internship**, Intel China Research Center, Beijing, China

- Improved the CE structural alignment algorithm for remote homology detection.

TRAININGS

2018 Scalable and Reproducible Structural Bioinformatics Workshop & Hackathon 2018, San Diego, CA

2015 Anton Workshop 2015, Pittsburgh, PA

2003 School of Parallel Computing, Chinese Academy of Science, Beijing, China

TEACHING AND MENTORING

2013 **Co-Mentor,** Undergraduate Research Opportunity Program (UROP), University of Michigan

- Coached an undergraduate student during his summer research project about computer-aided discovery of novel druggable pockets in heterotrimeric G proteins. Helped the student develop proper research strategies, master necessary techniques to conduct the research, and prepare a presentation about the results for a conference.

2003 **Teaching Assistant** (Statistical Physics), School of Physics, Peking University

- Instructed students on solving problems.
- Assisted the lecturer to grade course assignments and the final exam.

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

PROFESSIONAL MEMBERSHIP

2018–present American Chemical Society

2009–present Biophysical Society

2010–2012 Biophysical Society of Japan

SKILLS

OS	Linux, Windows
Software	Amber, Gromacs, AutoDock, Modeller, VMD, PyMol, etc.
Programming	R, C/C++, FORTRAN, Bash, Perl, Python, Tcl
Language	Mandarin Chinese, English

REVIEWER

Journals:

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

Conferences:

2017's Scientific Computing Day, Atlanta

PUBLICATIONS

*Peer-reviewed Journal Articles (*Joint-First; §Co-Corresponding)*

– 2018 –

1. **Yao XQ**[§], Momin M, and Hamelberg D[§]. Elucidating allosteric communications in proteins with difference contact network analysis. *J Chem Inf Molel* (2018) 58:1325-1330. DOI:10.1021/acs.jcim.8b00250
2. Rodriguez-Bussey I, **Yao XQ**, Shouaib AD, Lopez J, and Hamelberg D. Decoding allosteric communication pathways in cyclophilin A with a comparative analysis of perturbed conformational ensembles. *J Phys Chem B* (2018) 122:6528-6535. DOI:10.1021/acs.jpcb.8b03824
3. Momin MF, **Yao XQ**, Thor W, and Hamelberg D. Substrate sequence determines catalytic activities, domain-binding preferences, and allosteric mechanisms in Pin1. *J Phys Chem B* (2018) 122:6521-6527. DOI:10.1021/acs.jpcb.8b03819
4. 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. *ACS Catalysis* (2018) **8**:2375-2384. DOI:10.1021/acscatal.7b04263

– 2017 –

5. **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. DOI:10.1074/jbc.m117.807461
6. 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) 92:707-717. DOI:10.1124/mol.117.110130
7. 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. DOI:10.1016/j.molcel.2017.02.008
8. 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. DOI:10.1016/j.chembiol.2016.11.014

9. Jariwala S, Skjærven L, **Yao XQ**, and Grant BJ. Investigating protein sequence-structure-dynamics relationships with Bio3D-web. *J Vis Exp* (2017) 125:e55640. DOI:10.3791/55640

– 2016 –

10. **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. DOI:10.1021/acs.jpcb.6b01991
11. **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. DOI:10.1074/jbc.M115.702605
12. Skjærven L, Jariwala S, **Yao XQ**, and Grant BJ. Online interactive analysis of protein structure ensembles with Bio3D-web. *Bioinformatics* (2016) 32:3510-3512. DOI:10.1093/bioinformatics/btw482

– 2008-2015 –

13. 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. DOI:10.1016/j.bpj.2015.08.027
14. Skjaerven L, **Yao XQ**, Scarabelli G, and Grant BJ. Integrating protein structural dynamics and evolutionary analysis with Bio3D. *BMC Bioinformatics* (2014) 15:399. DOI:10.1186/s12859-014-0399-6
15. **Yao XQ** and Grant BJ. Domain-opening and dynamic coupling in the α-subunit of heterotrimeric G proteins. *Biophys J* (2013) 105:L08-L10. DOI:10.1016/j.bpj.2013.06.006
16. **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. DOI:10.1021/ja310548h
17. 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. DOI:10.1021/ct2001045
18. **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. DOI:10.1038/ncomms1116
    (The work was highlighted in public media: *Nikkei Business Daily*, *Nikkan Kogyo Shimbun*, and *Kyoto Shimbun*).
19. 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. DOI:10.1016/j.bbrc.2010.01.003
20. 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. DOI:10.3866/PKU.WHXB20100733
21. 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. DOI:10.1016/j.bbrc.2009.05.032
22. **Yao XQ** and She ZS. Key residue-dominated protein folding dynamics. *Biochem Biophys Res Comm* (2008) 373:64-68. DOI:10.1016/j.bbrc.2008.05.179

23. **Yao XQ**, Zhu HQ, and She ZS. A dynamic Bayesian network approach to protein secondary structure prediction. *BMC Bioinformatics* (2008) 9:49. DOI:10.1186/1471-2105-9-49

Talks

- "Elucidating allosteric communications in proteins with difference contact network analysis", ***The 256th ACS National Meeting & Exposition***, Boston (2018) *Accepted*
- "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

- Vu PJ, **Yao XQ**, Momin M, and Hamelberg D. Evolutionarily conserved and divergent residue-residue contact dynamics provide insights into the allosteric regulation of cyclophilins. *The9th Southeast Enzyme Conference*, Atlanta (2018)
- Vu PJ, **Yao XQ**, Momin M, and Hamelberg D. Evolutionarily conserved and divergent residue-residue contact dynamics provide insights into the allosteric regulation of cyclophilins. *The 255th ACS National Meeting & Exposition*, New Orleans (2018)
- Vu PJ, **Yao XQ**, Momin M, and Hamelberg D. Evolutionarily conserved and divergent residue-residue contact dynamics provide insights into the allosteric regulation of cyclophilins. *The 62nd Annual Meeting of Biophysical Society*, San Francisco (2018)

- **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.