Jiaye Guo

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EDUCATION

2012-Present **Ph.D. Candidate**
SUNY at Stony Brook, Stony Brook, NY

2008-2012 **Bachelor of Science, Biological Sciences**
Sichuan University, Chengdu, Sichuan, China

AWARDS AND HONORS

2015 Computing Research Association-Women (CRA-W) Grad Cohort Travel Award
2011 Annual Scholarship, Sichuan University
2010 Annual Scholarship, Sichuan University
2010 Outstanding Library Volunteer, Sichuan University
2009 Annual Scholarship, Sichuan University

RESEARCH EXPERIENCE

2013-Present **Graduate Research in Computational Structural Biology**
Advisor: Dr. Robert C. Rizzo, Dept. of Applied Math and Stats., SUNY at Stony Brook

- Develop a virtual screen protocol that incorporates bridging water molecules using solvated footprints
- Identify mutant-specific inhibitors targeting the kinase domain of HER2 as therapeutics for breast cancer
- Explore structural mechanisms of HER2 activation by HER3 in an asymmetric heterodimer using Gaussian accelerated MD simulations

2011-2012 **Undergraduate Research in Molecular Genetics**
Advisor: Dr. Xu Song, Dept. of Life Sciences, Sichuan University

- Purify human coagulation factor VII using affinity chromatography
- Characterize coagulation factor VII activity using *in vitro* assays

Summer 2011 **Undergraduate Research in Biophysics**
Advisor: Dr. Roy D. Welch, Dept. of Biology, Syracuse University

- Grow fluorescence-labeled cell cultures of the bacterium *Myxococcus xanthus*
- Make time-lapse movies of individual *Myxococcus xanthus* cell motion via fluorescence microscopy
- Develop a mathematical description of the fruiting body forming by *Myxococcus xanthus*

2010-2011 **Undergraduate Research in Plant Reproductive Biology**
Advisor: Dr. Danilo D. Fernando, Dept. of Environmental & Forest Biology, SUNY-ESF

- Clone an mi-RNA and the construct of the protein "Argonaute" using PCR
- Transform the cloned constructs into *Ginkgo biloba* germinated pollens via Agrobacterium

TEACHING EXPERIENCE

2016 **Teaching Assistant**
Dept. of Applied Mathematics and Statistics, SUNY at Stony Brook
AMS535: Introduction to Computational Structural Biology and Drug Design

2015 **Teaching Assistant**
Dept. of Applied Mathematics and Statistics, SUNY at Stony Brook
AMS536: Molecular Modeling of Biological Molecules

2013 **Teaching Assistant**
Dept. of Biochemistry and Cell Biology, SUNY at Stony Brook
BIO365: Biochemistry Laboratory

2013 **Teaching Assistant**
Dept. of Biochemistry and Cell Biology, SUNY at Stony Brook
BIO205: Fundamentals of Scientific Inquiry in the Biological Sciences IIA

OTHER EXPERIENCE / PROFESSIONAL MEMBERSHIP

2015 **Presider, 250th American Chemical Society National Meeting & Exposition, Boston, MA**

2014 **Presider, 247th American Chemical Society National Meeting & Exposition, Dallas, TX**

2013-Present **American Chemical Society**

2012-Present **New York Academy of Science**

ORAL / POSTER PRESENTATIONS

2017 **Guo, J.**; Rizzo, R. C. A Computational Approach to Energetically Identify Bridging Water Molecules and to Incorporate Them in Virtual Screens; 254th American Chemical Society National Meeting & Exposition, Washington, DC {Abstract & Poster (COMP-268)}

2017 **Guo, J.**; Rizzo, R. C. A Computational Approach to Identify and Incorporate Bridging Water Molecules in Drug-lead Discovery. Structural Biology Related to HIV/AIDS-2017 Meeting, Bethesda, MD {Abstract & Poster}

2016 **Guo, J.**; Rizzo, R. C. Developing Mutant-specific Inhibitors of HER2 Incorporating Bridging Water Molecules; 252nd American Chemical Society National Meeting & Exposition, Philadelphia, PA {Abstract & Poster (COMP-217)}

2016 **Guo, J.**; Rizzo, R. C. Identifying and incorporating water-mediated interactions in drug discovery. Structural Biology Related to HIV/AIDS-2016 Meeting, Bethesda, MD {Abstract & Poster}

2015 **Guo, J.** Footprint similarity scoring and ligand enrichment. AMS535: Introduction to Computational Structural Biology and Drug Design, SUNY at Stony Brook, Stony Brook, NY {Guest Lecture}

2015 **Guo, J.**; Rizzo, R. C. Inhibitor Development Targeting HER2 Incorporating Bridging Water Molecules; 250th American Chemical Society National Meeting & Exposition, Boston, MA {Abstract & Poster (COMP-308)}

2015 **Guo, J.**; Rizzo, R. C. Protocol development to include solvated molecular footprints in lead discovery; Structural Biology Related to HIV/AIDS-2015 Meeting, Bethesda, MD {Abstract & Poster}

2015 **Guo, J.**; Rizzo, R. C. Incorporating bridging-waters into structure-based drug design using molecular footprints; CRA-W Grad Cohort Workshop 2015, San Francisco, CA {Abstract & Poster}

2014	**Guo, J.** Footprint similarity scoring and ligand enrichment. AMS535: Introduction to Computational Structural Biology and Drug Design, SUNY at Stony Brook, Stony Brook, NY {Guest Lecture}
2014	**Guo, J.**; Rizzo, R. C. Incorporating bridging-waters into lead discovery using molecular footprints; Structural Biology Related to HIV/AIDS-2014 Meeting, Bethesda, MD {Abstract & Poster}
2014	**Guo, J.**; Rizzo, R. C. Structure-based drug design employing solvated molecular footprints; 247th American Chemical Society National Meeting & Exposition, Dallas, TX {Abstract & Poster (COMP-202)}
2013	**Guo, J.** Introduction to ligand enrichment and molecular footprints. AMS535: Introduction to Computational Structural Biology and Drug Design, SUNY at Stony Brook, Stony Brook, NY {Guest Lecture}

PUBLICATIONS

2018	**Guo, J.**; Collins, S.; Miller, W. T.; Rizzo, R. C. Coordination and Displacement of Bridging Waters using Solvated Footprints: Application to HER2. Manuscript prior to publication.
2014	Bahar, F.; Pratt-Szeliga, P. C.; Angus, S.; **Guo, J.**; Welch, R. D. Describing *Myxococcus xanthus* aggregation using Ostwald ripening equations for thin liquid films. *Sci Rep*. 4, 6376; DOI: 10.1038/srep06376 (2014).

TECHNICAL SKILLS

Platforms/Software: Linux/Unix, tcsh, bash, DOCK6, AMBER, VMD, UCSF-Chimera, MOE
Languages: Chinese (Native), English (Fluent), Python, C++