Ruo-Xu Gu

CONTACT INFORMATION

College of Life Sciences and Biotechnology,
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EDUCATION AND WORK EXPERIENCE

2020-present Tenure-track Associate Professor, Shanghai Jiao Tong University, China
2018-2020 AvH Postdoctoral Fellow, Max-Planck Institute for Biophysical Chemistry, Germany
2014-2018 CIHR, AIHS & CTPB Postdoctoral Fellow, University of Calgary, Canada
2007-2014 PhD in Biomedical Engineering, Shanghai Jiao Tong University, China
2003-2007 B.Sc. in Bioinformatics, Shanghai Jiao Tong University, China

RESEARCH FIELD

Molecular Modeling, Molecular Dynamics Simulation, Rational Drug Design,
Ion Channel, Lipid-Protein Interactions, Membrane Biophysics, Membrane Proteins

HONORS AND AWARDS

2019-2020 Alexander von Humboldt (AvH) Postdoctoral Fellowship
2015-2018 Canadian Institutes of Health Research (CIHR) Postdoctoral Fellowship
2015-2017 Alberta Innovates: Health Solutions (AIHS) Postdoctoral Fellowship
2016 The Excellent Doctoral Dissertation of Shanghai Municipality, China
2014 Create Training Program in Bionanomachines Postdoctoral Fellowship
2013 Arowana (JIN LONG YU) Scholarship
2012 National Academic Scholarship
2011 ZHAO ZHU MULAN Scholarship of Shanghai Jiao Tong University
2008 National Excellent Academic Scholarship
2006 Excellent Academic Scholarship of Shanghai Jiao Tong University
2004 SUMITOMO Scholarship of Shanghai Jiao Tong University

PUBLICATION

Peer Reviewed Journal Articles

23. **R.-X. Gu**, and B. L. de Groot. Lipid-Protein Interactions Modulate the Conformational Equilibrium of a Potassium Channel. ***Nature Communications***, 2020, 11:2162.

22. **R.-X. Gu**[#], S. Baoukina[#], and D. P. Tieleman. Phase Separation in Atomistic Simulations of Model Membranes. **Journal of the American Chemical Society,** 2020, 142 (6), 2844-2856.

21. **R.-X. Gu**, S. Baoukina, and D. P. Tieleman. Spontaneous Cholesterol Flip-Flop in Membranes

with Coexisting Domains. **Journal of Chemical Theory and Computation,** 2019, 15 (3), 2064-2070.

20. A. M. Grishin, K. R. Barber, **R.-X. Gu**, D. P. Tieleman, G. S. Shaw, and M. Cygler Regulation of Shigella Effector Kinase OspG through Modulation of Its Dynamic Properties. **Journal of Molecular Biology**, 2018, 430 (14), 2096-2112.

19. V. Corradi, E. Mendez-Villuendas, H. I. Ingólfsson, **R.-X. Gu**, I. Siuda, M. Melo, A. Moussatova, C. DeGagne, B. Sejdiu, G. Singh, T. Wassenaar, K. Delgado-Magnero, S. J. Marrink, and D. P. Tieleman. Lipid-Protein Interactions Are Unique Fingerprints for Membrane Proteins. **ACS Central Science**, 2018, 4 (6), 709-717**.**

18. V. Corradi, **R.-X. Gu**, P. Vergani, and D. P. Tieleman. Structure of Transmembrane Helix 8 and Possible Membrane Defects in CFTR. **Biophysical Journal**, 2018, 114 (8), 1751-1754.

17. E. Barreto-Ojeda, V. Corradi, **R.-X. Gu**, and D. P. Tieleman. Coarse-Grained Molecular Dynamics Simulations Reveal Lipid Access Pathways in P-glycoprotein. **Journal of General Physiology**, 2018, 150 (3), 417-429.

16. S. Hou, **R.-X. Gu***, and D. Q. Wei*. Inhibition of β-amyloid Channels with a Drug Candidate wgx-50 Revealed by Molecular Dynamics Simulations. **Journal of Chemical Information and Modeling,** 2017, 57 (11), 2811-2821*, **corresponding author.***

15. C. D. Li, Q. Xu, **R.-X. Gu**, J. Qu, and D. Q. Wei. The Dynamic Binding of Cholesterol to the Multiple Sites of C99: as Revealed by Coarsed-Grained and All-Atom Simulations. **Physical Chemistry Chemical Physics**, 2017, 19 (5), 3845-3856.

14. **R.-X. Gu**, H. I. Ingólfsson, A. H. de Vries, S. J. Marrink, and D. P. Tieleman. Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. **Journal of Physical Chemistry B**, 2017, 117 (20), 6042-6051.

13. T. Ulaganathan, R. Shi, D. Yao, **R.-X. Gu**, Y. Li, M. L. Garron, M., D. P. Tieleman, E. Sterner, G. Li, L. Li, R.J. Linhardt, and M. Cygler. Conformational Flexibility of Heparinases from PL12 family: Crystal Structure and Substrate Specificity of Heparinase III from *Bacteroides thetaiotaomicron (BT4657)*. **Glycobiology**, 2017, 27 (2), 176-187.

12. **R.-X. Gu**, V. Corradi, G. Singh, H. G. Choudhury, K. Beis, and D. P. Tieleman. Conformational Changes of the Antibacterial Peptide ATP Binding Cassette Transporter McjD Revealed by Molecular Dynamics Simulations. **Biochemistry**, 2015, 54 (38), 5989-5998.

11. H. M. Fan, **R.-X. Gu**, Y. J. Wang, Y. L. Pi, Y. H. Zhang, Q. Xu, and D. Q. Wei. Destabilization of Alzheimer's Aβ42 Protofibrils with a Novel Drug Candidate wgx-50 by Molecular Dynamics Simulations. **Journal of Physical Chemistry B**, 2015, 119 (34), 11196-11202.

10. Y. K. Wang, D. Q Wei, **R.-X. Gu**, H. M. Fan, and J. Ulmschneider. Applications of Rare Event Dynamics on the Free Energy Calculations for Membrane Protein Systems. **Canadian Journal of Chemistry**, 2013, 91 (9), 769-774.

9. **R.-X. Gu**, L. A. Liu, and D. Q. Wei. Structural and Energetic Analysis of Drug Inhibition of the Influenza A M2 Proton Channel. **Trends in Pharmacological Sciences**, 2013, 34 (10), 571-580.

8. **R.-X. Gu**, L. A. Liu, Y. H. Wang, Q. Xu, and D. Q. Wei. Structural Comparison of the Wild-Type and Drug-Resistant Mutants of the Influenza A M2 Proton Channel by Molecular Dynamics Simulations. **Journal of Physical Chemistry B**, 2013, 117 (20), 6042-6051.

7. S. G. Chen[#], **R.-X. Gu**[#]*, H. Dai, and D. Q. Wei. Virtual Screening for α7 Nicotinic Acetylcholine Receptor for Treatment of Alzheimer's Disease. **Journal of Molecular Graphics & Modeling**, 2013, 39, 98-107, ***co-first author and corresponding author***.

6. **R.-X. Gu**, L. A. Liu, D. Q. Wei, J. G. Du, L. Liu, and H. Liu. Free Energy Calculations on the Two Drug Binding Sites in the M2 Proton Channel. **Journal of the American Chemical Society**, 2011, 133 (28), 10817-10825.

5. **R.-X. Gu**, Y. Q. Zhong, and D. Q. Wei. Structural Basis of Agonist Selectivity for Different n AChR Subtypes: Insights from Crystal Structures, Mutation Experiments and Molecular Simulations. **Current Pharmaceutical Design**, 2011, 17 (17), 1652-1662**.**

4. H. R. Arias[#], **R.-X. Gu**[#], D. Feuerbach, B. B. Guo, Y. Ye, and D. Q. Wei. Novel Positive Allosteric Modulators of the Human α7 Nicotinic Acetylcholine Receptor. **Biochemistry**, 2011, 50 (23), 5263-5278, ***co-first author.***

3. H. M. Lv, X. L. Guo, **R.-X. Gu**, and D. Q. Wei. Free Energy Calculations and Binding Analysis of Two Potential Anti-Influenza Drugs with Polymerase Basic Protein-2 (BP2). **Protein and Peptide letters**, 2011, 18(10), 1002-1009.

2. H. R. Arias[#], **R.-X. Gu**[#], D. Feuerbach, and D. Q. Wei. Different Interaction between the Agonist JN403 and the Competitive Antagonist Methyllycaconitine with the Human α7 Nicotinic Acetylcholine Receptor. **Biochemistry**, 2010, 49 (19), 4169-4180, ***co-first author.***

1. **R.-X. Gu**, H. Gu, Z. Y. Xie, J. F. Wang, H. R. Arias, D. Q. Wei, and K. C. Chou. Possible Drug Candidates for Alzheimer's Disease Deduced from Studying their Binding Interactions with α7 Nicotinic Acetylcholine Receptor. **Medicinal Chemistry**, 2009, 5 (3), 250-262.

Book Chapters

2. H. M. Fan, **R.-X. Gu**, and D. Q. Wei. The α7 nAChR Selective Agonists as Drug Candidates for Alzheimer's Disease. **Advance in Structural Bioinformatics**, Volume 827, 2014, 353-365.

1. **R.-X. Gu**, L. A. Liu, and D. Q. Wei. Drug Inhibition and Proton Conduction Mechanisms of the Influenza A M2 Proton Channel. **Advance in Structural Bioinformatics**, Volume 827, 2014, 205-226.

SERVICE

Guest Editor

Zunnan Huang and **Ruo-Xu Gu**, "Development and Application of Computational Methods in Biology and Medicine", **Current Medicinal Chemistry**, 2019, 62 (42).

Zunnan Huang, **Ruo-Xu Gu**, and Xiao Jun Yao, "Computational Approaches in Drug Discovery and Precision Medicine", **Frontiers in Chemistry**, 2020, in process.

Review manuscripts for *Journal of the American Chemical Society*, *Journal of Chemical Information and Modeling*, *Journal of Physical Chemistry B*, *Biophysical Journal*, *PLoS one*, *Current Medicinal Chemistry, Current Pharmaceutical Design*.

TEACHING EXPERIENCE

Teaching Assistant, Physics, 2008, Shanghai Jiao Tong University, China

PROFESSIONAL ACTIVITIES

2017 Poster presentation at the Biophysical Society 61th Annual Meeting, New Orleans

2016 Poster presentation at the 4th Theory and Applications of Computational Chemistry Conference, Seattle, US

2016 Poster Presentation at the Biophysical Society 60th Annual Meeting, Los Angeles

2015 Poster Presentation at the 3nd Protein Structure Function and Malfunction Conference, Saskatoon, Canada

2015 Poster Presentation at the Biophysical Society 59th Annual Meeting, Baltimore

2014 Oral Presentation at the 2nd Protein Structure Function and Malfunction Conference, Saskatoon, Canada

2011 Oral Presentation at the 28th Annual Symposium of Chinese Chemical Society, Chengdu

2011 Oral Presentation at the International Conference of the Computational and Systems Biology, Shanghai

2010 Poster Presentation at the International Conference of the Computational and Systems Biology, Hangzhou