

QIAN WANG

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EDUCATION

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| ❖ M.S., Master of Computer and Information Technology, University of Pennsylvania | 01/2022 – present |
| ❖ Ph.D., Biochemistry, The Graduate Center, City University of New York (CUNY) | 08/2010 – 09/2017 |
| ❖ B.S., Biotechnology, Yantai University, Yantai, Shandong, P.R. China | 09/2005 – 06/2009 |

PUBLICATIONS

- ❖ **Qian Wang**, Aleksey Aleshintsev, Kamal Rai, Eric Jin, and Rupal Gupta. "Proton Transfer via Arginine with Suppressed pKa Mediates Catalysis by Gentisate and Salicylate Dioxygenase." *The Journal of Physical Chemistry B* (2024): 128 (28), 6797–6805.
- ❖ **Qian Wang**, Christopher DiForte, Aleksey Aleshintsev, Gianna Elci, Shibani Bhattacharya, Angelo Bongiorno, and Rupal Gupta. "Calcium mediated static and dynamic allostery in S100A12: Implications for target recognition by S100 proteins." *Protein Science* 33, no. 4 (2024): e4955.
- ❖ **Qian Wang**, Hanbin Li, Uran Bujupi, Janosch Gröning, Andreas Stolz, Angelo Bongiorno, and Rupal Gupta. "Oxygen Activation in Aromatic Ring Cleaving Salicylate Dioxygenase: Detection of Reaction Intermediates with a Nitro-substituted Substrate Analog." *ChemBioChem* (2024): e202400023.
- ❖ Jianqin Zhuang, **Qian Wang**, and Rupal Gupta. "Applications of ¹⁷O and ⁵¹V NMR in inorganic and bioinorganic chemistry." (2023): 35-61.
- ❖ **Qian Wang**, Deniz Kuci, Shibani Bhattacharya, Jodi A. Hadden-Perilla, and Rupal Gupta. "Dynamic regulation of Zn (II) sequestration by calgranulin C." *Protein Science* 31, no. 9 (2022): e4403.
- ❖ **Qian Wang**, Aleksey Aleshintsev, Aneesha N. Jose, James M. Aramini, and Rupal Gupta. "Calcium regulates S100A12 zinc sequestration by limiting structural variations." *ChemBioChem* 21, no. 9 (2020): 1372-1382.
- ❖ **Qian Wang**, Aleksey Aleshintsev, David Bolton, Jianqin Zhuang, Michael Brenowitz, and Rupal Gupta. "Ca (II) and Zn (II) cooperate to modulate the structure and self-assembly of S100A12." *Biochemistry* 58, no. 17 (2019): 2269-2281.
- ❖ **Qian Wang**, Samar Rizk, Cédric Bernard, May Poh Lai, David Kam, Judith Storch, and Ruth E. Stark. "Protocols and pitfalls in obtaining fatty acid-binding proteins for biophysical studies of ligand-protein and protein-protein interactions." *Biochemistry and Biophysics Reports* 10 (2017): 318-324.
- ❖ Feng, Guoying, Xiaobo Xu, **Qian Wang**, Zhen Liu, Zhenzhong Li, and Guixiang Liu. "The protective effects of calcitonin gene-related peptide on gastric mucosa injury after cerebral ischemia reperfusion in rats." *Regulatory Peptides* 160, no. 1-3 (2010): 121-128.
- ❖ Cai, Heng, Xiaobo Xu, Zhen Liu, **Qian Wang**, Guoying Feng, Yizhao Li, Chunsheng Xu, Guixiang Liu, and Zhenzhong Li. "The effects of calcitonin gene-related peptide on bFGF and AQP4 expression after focal cerebral ischemia reperfusion in rats." *Die Pharmazie-An International Journal of Pharmaceutical Sciences* 65, no. 4 (2010): 274-278.
- ❖ Feng, Guoying, **Qian Wang**, Xiaobo Xu, Zhen Liu, Zhenzhong Li, and Guixiang Liu. "The protective effects of calcitonin gene-related peptide on gastric mucosa injury of gastric ischemia reperfusion in rats." *Immunopharmacology and Immunotoxicology* 33, no. 1 (2011): 84-89.

RESEARCH EXPERIENCE

GRADUATE REASERCH

Sept 2011 – June 2017

Characterized the structure, function, and interactions of adipocyte fatty acid-binding protein (AFABP/FABP4) to understand its role in lipid metabolism, insulin resistance, and obesity.

- ❖ Optimized a robust protocol for isolating AFABP in both its liganded and ligand-free forms, employing hydrophobically functionalized hydroxypropyl dextran beads to remove bound lipids.
- ❖ Validated the purity and structural integrity of isolated AFABP using two-dimensional NMR spectroscopy, ensuring suitability for downstream biochemical and biophysical studies.
- ❖ Investigated the oligomerization states of AFABP under physiological conditions, identifying factors that promote or inhibit the formation of disulfide-linked homodimers through gel filtration chromatography.
- ❖ Improved the protocol for preparing peroxisome proliferator-activated receptor gamma (PPAR γ), increasing its yield from less than 1 mg per liter of LB culture to over 50 mg per liter of LB culture. This enhancement significantly facilitates in vitro studies of PPAR γ .

- ❖ Provided critical insights into the self-association behavior of AFABP and established conditions to modulate dimerization, forming a basis for studying its interactions with nuclear receptors such as PPAR γ .
- ❖ Supported future research into the role of AFABP in lipid transport and its contribution to metabolic disorders by developing scalable and reproducible methodologies.

POSTDOCTORAL REASERCH

Feb 2020 - present

Investigated the catalytic mechanisms of cupin dioxygenases, including salicylate 1,2-dioxygenase (SDO) and gentisate 1,2-dioxygenase (GDO), which are key enzymes in the aerobic degradation of aromatic rings and global carbon cycling.

- ❖ Demonstrated the role of a proton shuffler in catalysis by these enzymes, identifying a conserved arginine residue as the proton donor via pH-dependent Michaelis-Menten analysis and thermodynamic studies ($\Delta H_{ion}^{\circ} = 51$ kJ/mol).
- ❖ Explored the effect of the 3-histidine ferrous binding scaffold in GDOs, proposing its role in modulating the arginine pKa through mutational analysis.
- ❖ Characterized transient reaction intermediates of SDO using a substrate analog (3-nitrogentisate), revealing a 500-fold reduction in enzymatic k_{cat} and enabling kinetic and spectroscopic insights into dioxygen binding and intermediate formation.
- ❖ Determined that dioxygen binding to the iron cofactor occurs at a rate of $5.9 \times 10^3 \text{ M}^{-1}\text{s}^{-1}$, slower than other dioxygenases, and identified distinct chromophoric signatures for intermediates critical to the reaction cycle.

POSTDOCTORAL REASERCH

Oct 2017 - present

Explored the structure-function relationships and metal-binding dynamics of S100 proteins, including S100A12 (Calgranulin C), to understand their roles in immune response and antimicrobial activity.

- ❖ Investigated the cooperativity between the two calcium-binding EF-hand motifs in S100A12 using solution-state NMR spectroscopy and designed mutants (N63A, E31A) to selectively bind calcium at individual EF loops. Demonstrated that EF-II loop binding is the principal trigger for conformational changes from the 'closed' apo to the 'open' calcium-bound state.
- ❖ Measured amide nitrogen relaxation rates (R_1 , R_2 , and ^{15}N - $\{^1\text{H}\}$ NOE) and performed molecular dynamics (MD) simulations to reveal dynamic regulatory roles of EF-I loop binding and its impact on polypeptide fluctuations.
- ❖ Characterized the pH- and calcium-dependent modulation of zinc sequestration by S100A12, showing that calcium binding enhances zinc-binding affinity under acidic conditions, critical for antimicrobial activity during neutrophil activation.
- ❖ Utilized ^{15}N and ^{13}C CPMG dispersion experiments to map pH-dependent conformational exchanges in S100A12's EF-hand motifs and linker regions, uncovering a pH-regulated dynamic equilibrium of "closed" and partially "open" sidechain configurations in the zinc-binding site.
- ❖ Demonstrated that calcium and zinc binding cooperate to induce reversible self-assembly of S100A12, with conformational changes in helix II and the hinge domain affecting interactions with target proteins, such as the receptor for advanced glycation end products (RAGE), during inflammatory responses.
- ❖ Explored how metal-binding dynamics contribute to antimicrobial activity, chemotaxis, and modulation of inflammatory pathways through structural perturbations and interaction sites.

INVITED TALKS

- ❖ Invited by New York Structural Biological Center (NYSBC) October 2019

TECHNICAL SKILLS

- ❖ **Advanced Instrumentation and Techniques:** Proficient in nuclear magnetic resonance (NMR)

spectroscopy for structural and dynamic studies of biomolecules, including isotope-labeled protein samples.

- ❖ **Microscopy Expertise:** Skilled in fluorescence microscopy for imaging and analysis of biological systems.
- ❖ **Protein Expression and Purification:** Extensive experience in heterologous protein expression and purification from both *E. coli* and mammalian cell systems, including isotope labeling as required.
- ❖ **Problem-Solving and Troubleshooting:** Proven ability to creatively address experimental challenges and resolve technical issues efficiently. For example, suggested increasing temperature during CPMG relaxation experiments to enhance molecular dynamics, achieving better resolution for accurate parameter fitting.
- ❖ **Strong Execution Capability:** Demonstrated expertise in managing multiple projects simultaneously while training an average of three Ph.D. and undergraduate students concurrently. Consistently delivered high-quality results, meeting deadlines for preliminary data and final publications without requiring extensions.

TEACHING EXPERIENCE

Research Training Coordinator, College of Staten Island 11/2017 – present

- ❖ Trained over 10 undergraduate students, 3 Ph. D. candidates and 6 Ph.D. rotation students on implementing honor thesis or Ph.D. program.

STEM Education Facilitator, College of Staten Island 07/2019 – 07/2024

- ❖ Introduced and mentored over total 60 local high school and undergraduate students, fostering their passion for science and encouraging them to pursue scientific careers.

Adjunct Lecturer, General Physics, Hostos Community College 09/2015 – 05/2017

- ❖ Independently designed lectures to 30 undergraduate students on the principles of general physics.
- ❖ Instructed the 1.5-hour fundamental physics experiments for courses.
- ❖ Led the recitation of course with quizzes and practices.

Tutor, Biochemistry, General Chem., Physical Chem., College of Staten Island 11/2017 – 06/2018

- ❖ Tutored undergraduate students on Biochemistry, General Chemistry, Physical Chemistry and Inorganic Chemistry, including lecture assignments and lab reports.

Adjunct Lecturer, Inorganic Chemistry, College of Staten Island 01/2018 – 05/2018

- ❖ Instructed undergraduate students on Inorganic Chemistry lab, including compound synthesis, chemical kinetics study and product analysis by using UV-Vis, IR, MS or NMR spectroscopy.

Teaching Adjunct, General Chemistry II, The City College of New York 09/2012 – 06/2017

- ❖ Instructed 20 undergraduate students on the 3-hour 10 fundamental lab sections about Colligative Properties, thermodynamics, enzyme kinetics, electrochemistry and so forth.

Research Training Coordinator, The City College of New York 06/2011 – 06/2017

- ❖ Trained 3 undergraduates, high-school volunteers and 1 junior Ph.D. student for their independent study or Ph.D. program.

Lab Assistant, Qingdao Institute Bioenergy and Bioprocess Technique, P.R. China 09/2009 – 06/2010

- ❖ Maintained the microbiological instruments i.e. incubator, sterile work hood, sterilizer, PCR amplification instrument, electrophoresis, and micro-pulser.
- ❖ Trained the fresh graduate students to use the lab instrument.