TIANYIN(TIM) QIU

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EDUCATION

- **YALE UNIVERSITY Year:** 2020 – 2025 (Expected)
  Doctor of Philosophy (Ongoing) – Theoretical Chemistry
- **UNIVERSITY OF CALIFORNIA, IRVINE Year:** 2016 – 2020
  Bachelor of Science – Chemistry with Concentration in Computational & Theoretical Chemistry

RESEARCH EXPERIENCE

- **UNDERGRADUATE RESEARCHER** – University of California, Irvine
  Luo Lab (Department of Molecular Biology & Biochemistry) | Jan 2018 – Present
  Developed a GPU-accelerated MM-PBSA free energy calculation method for small ligands on biomacromolecules. Applied heterogenous implicit membrane models for more accurately calculating the binding free energies of charged ligands in GPCR membrane proteins
  Tsai Lab (Department of Molecular Biology & Biochemistry) | Jan 2019 – Present
  Applied molecular docking, molecular dynamics, and MM-PBSA to study the catalytic mechanism of Actinorhodin Polyketide Ketoreductase (ActKR)

PUBLICATIONS

- Greene, D., Qi, R., Nguyen, R., **Qiu, T.**, & Luo, R. (2019). Heterogeneous Dielectric Implicit Membrane Model for the Calculation of MMPBSA Binding Free Energies. *Journal of Chemical Information and Modeling*. doi: 10.1021/acs.jcim.9b00363.
- Wei, H., Luo, A., **Qiu, T.**, Luo, R. & Qi, R. (2019) Improved Poisson–Boltzmann Methods for High-Performance Computing. *Journal of Chemical Theory and Computation*. doi: 10.1021/acs.jctc.9b00602.
- **Qiu, T.** & Tsai, S. et al. (2019) Dissecting The Regiospecificity of Aromatic Polypeptide Ketoreductase Using Molecular Dynamic Simulations. (Manuscript submitted)
- **Qiu, T.**, & Luo, R. (2019) Computational Analysis of the Dimer Interface of p53 Bound to DNA (Poster published in ACS National Meeting & Expo 2019 COMP CHEM poster session)

SKILLS

- **Programming languages:** Python, Fortran90, Bash shell script, LATEX
- **Simulation Software:** Amber 18, Gaussian 09

HONORS & AWARDS

- **Allergan Undergraduate Research Program**   2019 Summer
  -Only award less than ten students each year
- **Summer Undergraduate Research Fellowship (SURP)**   2018 Summer, 2019 Summer
  -Awarded for two consecutive years
- **Undergraduate Research Opportunities Fellowship (UROP)**   2018 Spring – 2019 Winter
  -Awarded for three consecutive quarters
- **Phi Beta Kappa Member**   2019 – Present
  -Only for first 2 % of junior students by academic performance
- **Dean's Honor List**   2017 Winter – 2019 Spring

VOLUNTEER EXPERIENCE

- **Biological Sciences International Student Association (BISA)** – Irvine, CA
  Social Media Chair | July 2018 – Present