

## TIANYIN(TIM) QIU

Address: 275 Winchester Avenue, Apt 217, New Haven, CT 06511

Tel: (949) 344-0757 Email: tianyin.qiu@yale.edu

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## EDUCATION

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- **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
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## RESEARCH EXPERIENCE

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- **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 heterogeneous 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)
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## PUBLICATIONS

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- 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)
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## SKILLS

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- **Programming languages:** Python, Fortran90, Bash shell script, L<sup>A</sup>T<sub>E</sub>X
  - **Simulation Software:** Amber 18, Gaussian 09
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## HONORS & AWARDS

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- **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
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## VOLUNTEER EXPERIENCE

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