Hao Tian

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EDUCATION

Southern Methodist University, Dallas, TX — Aug. 2019 – May 2023

- Ph.D. in Theoretical and Computational Chemistry, GPA: 4.0 / 4.0
- Core courses: Statistical Thermodynamics, Advanced Computational Chemistry, Machine Learning and Neural Networks, Mathematical Statistics
- Thesis title: Exploring Protein Conformations and Functions Through Molecular Dynamics Simulations and Machine Learning

Georgia Institute of Technology, Atlanta, GA — Aug. 2020 – May 2023

- Online M.S. in Computer Science, GPA: 4.0 / 4.0
- Core courses: Database Systems Concepts and Design, Computer Networks, Graduate Introduction to Operating Systems, Introduction to Graduate Algorithms, Software Architecture and Design

Beijing University of Chemical Technology, Beijing, China — Aug. 2015 – Jun. 2019

- B.Eng. in Chemical Engineering, GPA: 3.49 / 4.33

TECH STACK

- **Languages**: Python, Java, C, C++, HTML, CSS, JavaScript, PHP
- **Toolkits & Frameworks**: Linux, Docker, Git, MySQL, Django, Bootstrap, RESTful API
- **Machine Learning**: Scikit-learn, Tensorflow (Keras), PyTorch

EXPERIENCE

Software Engineer Intern — **Meta** (Facebook), Menlo Park, CA — May 2022 – Aug. 2022

- Implemented a relay IP to real IP mapping service in Ads identity prediction for iOS 15 privacy mitigation.
- Wrote 3k+ lines of PHP codes for service implementation and 2k+ lines of SQL (Presto) for impact evaluation.
- Improved IP coverage by 2.5%, identity match rate by 11% in iOS 15.5 and 3% in the overall Meta Pixel traffic, leading to 1.7% offsite conversion gain and 0.08% of incremental revenue.
- Published one internal technical post about viewer context which leads to a team Better Engineering project.

Graduate Research Assistant — **Southern Methodist University**, Dallas, TX — Aug. 2019 – May 2023

- Developed machine learning models on high-performance computing (HPC) clusters with SLRUM scheduler.
- Launched a web server (40k+ visits) with Django for biology prediction, supporting job submission and protein visualization, with web pages written in HTML / CSS / Javascript and improved UI using Bootstrap.
- Act as the group's Tech Lead in leading and designing research directions and writing funding proposals.
- Initiated automated and customized development workflow with CI / CD via GitHub Actions.

PUBLICATIONS

Google Scholar link: https://scholar.google.com/citations?user=X7ZR8J0AAAAJ

16. **Tian, H.**, Xiao, S., Jiang, X., & Tao, P. (2023). PASSerRank: Prediction of Allosteric Sites with Learning to Rank. *Artificial Intelligence Chemistry*, accepted.
15. **Tian, H.**, Xiao, S., Jiang, X., & Tao, P. (2023). PASSer: Fast and Accurate Prediction of Protein Allosteric Sites. *Nucleic Acids Research*, gkad303.
14. Li, H., **Tian, H.**, Chen, Y., Xiao, S., Zhao, X., Gao, Y., & Zhang, L. (2023). Analyzing and Predicting the Viscosity of Polymer Nanocomposites in the Conditions of Temperature, Shear Rate, and Nanoparticle Loading with Molecular Dynamics Simulations and Machine Learning. The Journal of Physical Chemistry B, in press.
13. Xiao, S., Song, Z., **Tian, H.**, & Tao, P. (2023). Assessments of Variational Autoencoder in Protein Conformation Exploration. *Journal of Computational Biophysics and Chemistry*, 22, 1-13.
12. Yin, C., Song, Z., **Tian, H.**, Palzkill, T., & Tao, P. (2023). Unveiling the structural features that regulate carbapenem deacylation in KPC-2 through QM/MM and interpretable machine learning. *Physical Chemistry Chemical Physics*, 25(2), 1349-1362.
11. Krishnan, K., **Tian, H.**, Tao, P., & Verkhivker, G. M. (2022). Probing conformational landscapes and mechanisms of allosteric communication in the functional states of the ABL kinase domain using multiscale simulations and network-based mutational profiling of allosteric residue potentials. *The Journal of Chemical Physics*, 157(24), 245101.
10. **Tian, H.**, Jiang, X., Xiao, S., La Force, H., Larson, E. C., & Tao, P. (2022). LAST: Latent Space-Assisted Adaptive Sampling for Protein Trajectories. *Journal of Chemical Information and Modeling*, 63(1), 67-75.
9. **Tian, H.**, Ketkar, R., & Tao, P. (2022). ADMETboost: a web server for accurate ADMET prediction. *Journal of Molecular Modeling*, 28(12), 1-6.
8. Song, Z., Trozzi, F., **Tian, H.**, Yin, C., & Tao, P. (2022). Mechanistic insights into enzyme catalysis from explaining machine-learned quantum mechanical and molecular mechanical minimum energy pathways. *ACS Physical Chemistry Au*, 2(4), 316-330.
7. Xiao, S., **Tian, H.**, & Tao, P. (2022). PASSer2. 0: accurate prediction of protein allosteric sites through automated machine learning. *Frontiers in Molecular Biosciences*, 9.
6. **Tian, H.**, & Tao, P. (2021). Deciphering the protein motion of S1 subunit in SARS-CoV-2 spike glycoprotein through integrated computational methods. *Journal of Biomolecular Structure and Dynamics*, 39(17), 6705-6712.
5. **Tian, H.**, Jiang, X., Trozzi, F., Xiao, S., Larson, E. C., & Tao, P. (2021). Explore protein conformational space with variational autoencoder. *Frontiers in Molecular Biosciences*, 8, 781635.
4. **Tian, H.**, Jiang, X., & Tao, P. (2021). PASSer: Prediction of allosteric sites server. *Machine Learning: Science and Technology*, 2(3), 035015.
3. Song, Z., Zhou, H., **Tian, H.**, Wang, X., & Tao, P. (2020). Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. *Communications Chemistry*, 3(1), 134.
2. **Tian, H.**, Trozzi, F., Zoltowski, B. D., & Tao, P. (2020). Deciphering the allosteric process of the Phaeodactylum tricornutum Aureochrome 1a LOV domain. *The Journal of Physical Chemistry B*, 124(41), 8960-8972.
1. **Tian, H.**, & Tao, P. (2020). ivis Dimensionality Reduction Framework for Biomacromolecular Simulations. *Journal of Chemical Information and Modeling*, 60(10), 4569-4581.

PRESENTATIONS

Oral

- Prediction of Allosteric Sites Through Ensembled Learning
  ACS Spring 2021, Apr. 2021
- ivis Dimensionality Reduction Method for Macromolecular Simulations
  ACS Spring 2021, Apr. 2021
- Machine Learning Framework for Deciphering the Allosteric Process of Circadian Clock Protein
  Invited seminar talk, Department of Chemistry and Biochemistry, The University of Oklahoma, Nov. 2020

Poster

- Iterative expansion of protein conformational space with variational autoencoder
  ACS Fall 2022, Aug. 2022
- Exploration of protein conformational space with variational autoencoder
  ACS Spring 2022, Mar. 2022

AWARDS

- Research Achievement Award, Southern Methodist University, Dec. 2022
- Chemical Computing Group Excellence Award for Graduate Students, American Chemical Society, Computers In Chemistry division, Apr. 2022 (only 5 awardees in each meeting)
- Research and Innovation Week Dean's Award, Southern Methodist University, May 2021 & Apr. 2022
- Graduate Research Assistant Award, Southern Methodist University, May 2021
- Outstanding Teaching Assistant, Southern Methodist University, May 2020

SERVICES

Journal Reviewer

- BioMedInformatics
- Biomolecules
- Cancers
- Computational and Structural Biotechnology Journal
- Frontiers in Cardiovascular Medicine
- International Journal of Molecular Sciences
- Living Journal of Computational Molecular Science
- Machine Learning: Science and Technology
- Molecules

Conference and Workshop Reviewer

- NeurIPS 2022 Workshop AI4Science