ODIN ZHANG

(HAOTIAN ZHANG)

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EDUCATION

Zhejiang University — Hangzhou, China
B.S in Pharmaceutical science & B.S in Physics, advised by **Tingjun Hou** — 2018.8 –2022.6

- GPA: 3.85/4.00
- First Prize in China Undergraduate Physics Tournament (Top 0.1%)
- Selected to Morningside Cultural China Scholars Program
- 2020 Top Ten College Students in the College of Pharmacy (TOP 0.8%)
- Four First Prize in the 16th University Sports Games Of Zhejiang Province

RESEARCH INTERESTS

AI4Science; Generative Model; Computer-aided Drug Design; Molecular Dynamics

RESEARCH EXPERIENCE

Carbon Silicon AI (a start-up) — Hangzhou, China
Senior DL-Engineer, leading a 10-people group — 2022.05– Present

- Developed molecular conformation generation algorithms, the main product is **SDEGen.**
- Developed 3D pocket-aware drug design models, the main products are **ResGen** and **SurfGen.**
- Developed the first unified deep lead optimization framework, the main product is **Delete.**
- Developed protein-ligand binding conformation prediction model, the main product is **KarmaDock**
- Responsible for the molecular generation direction.

Drug Design and Computational Biology Group — Hangzhou, China
Research Assistant — 2019.03– Present

- Participated in binding affinity prediction program, giving a talk on the ACS graduate Branch.
- Conducted the undergraduate thesis about conformation generation, the first article in the group accepted by *Chemical Science.*
- Conducted the undergraduate training program, performing a study about GPCR-specific scoring function.
- Performed molecular dynamics to observe the binding mechanism of triazolotriazine to the A2A adenosine receptor, cooperated with the Insititute of Mathematical Physics, Chinese Academy of Sciences.
- Mentored and trained 3 undergraduate students
- Selected as a teaching assistant for Calculus and Physical Chemistry.

Center of Modern Physics — Hangzhou, China
Undergraduate Thesis — 2022.01 –2022.07

- Conducted the undergraduate thesis about combining generative modeling with traditional computational tools.
- Performed the Coarse-Grained molecular dynamics (CGMD) to observe the self-assembly of nanoparticles, suggesting the conclusion of wet experiments.
- Performed Atomic MD and CGMD to rational design nanomedicine.

LEADERSHIP/TEAMWORK EXPERIENCE

Zhejiang Lab (Province Key Lab, https://en.zhejianglab.com/) — Hangzhou, China
Consultant of A1-aided Drug Discovery — 2022.06– Present

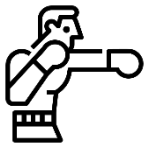
- Proposed specific chemical applications for intelligent reaction prediction
- Cooperated with a wet-experiment group on nucleic acid drug design.
- Cooperated on the method for drug design targeting protein with metal ions.
- Advised potential improvement strategies for docking programs.
- Assisted senior researchers in applying for state funding.

Artificial Intelligence Club Hangzhou, China
Director of Academic Department 2021.03– Present

- Organized a seminar (~60 people) for *Pattern and Recognition and machine learning.*
- Established and maintained relationships with companies seeking job opportunities.
- Organized club members a participate in machine learning competitions.

OTHER ACTIVITIES

- President of Jingwu Club of Zhejiang University (the club of boxing), 2019-2020.
- Leader Member of Lingyun Outdoor Sports Club, 2021-2022.
- Annual Meeting of Chinese Chemical Society, 2022.
- ACS annual graduate forum spring poster, 2022. (in undergraduate duration)



PUBLICATIONS

1. **Zhang, H.**, et al. ResGen: A Pocket-aware 3D Molecular Generation Model Based on Parallel Multi-scale Modeling, ***Nature Machine Intelligence***, *5*, 1020–1030 (2023). Code
2. **Zhang, H.**, et al. SurfGen: Learning on Topological Surface and Geometric Structure for 3D Molecular Generation, ***Nature Computational Science***, 3, 849–859 (2023). Code
3. **Zhang, H.**, Graph Neural Network as a Cornerstone in Modern Drug Discovery. ***Chemical Reviews***, proposal accepted.
4. Zhang, X.*, **Zhang, H.***, et al. KarmaDock: a deep learning paradigm for ultra-large library docking with fast speed and high accuracy. ***Nature Computational Science***, *3*, 739–740 (2023). Code
5. **Zhang, H.,** et al. Delete: Deep Lead Optimization Enveloped in Protein Pocket through Deleting Strategy combined with an E(3)-equivariant Framework ——When you face some problems in drug discovery, just delete! ***Nature Communications***, major revision. Code
6. Pan, P.*, Chen, S.*, **Zhang, H.***, Structure-based Molecular Generation: A New Paradigm Enables Efficient Design of Potent CLIP1-LTK Inhibitors. Submitted to *Nature Biomedical Engineering.*
7. **Zhang, H.**, Li, S., Zhang, J., Wang, Z., Wang, J., Jiang, D., ... & Hou, T. (2023). SDEGen: learning to evolve molecular conformations from thermodynamic noise for conformation generation. ***Chemical Science***, *14*(6), 1557-1568. Code
8. **Zhang, H.**, Zhang, J., Zhao, H., Jiang, D., & Deng, Y. (2023). Infinite Physical Monkey: Do Deep Learning Methods Really Perform Better in Conformation Generation? *bioRxiv*, 2023-03. Code
9. **Zhang, H.**, Deep Lead Optimization via a View of Constrained Molecular Generation: from Goals to Tools.
10. Wang, T.*, Zhang, X.*, **Zhang, H.***, et al. Highly accurate and efficient deep learning paradigm for full-atom protein loop modeling with KarmaLoop. ***Nature Machine Intelligence***, major revision. Code
11. Zhang, J.*, **Zhang, H.*,** Qin, Z., Kang, Y., Hong, X., & Hou, T. (2023). Quasiclassical Trajectory Simulation as a Protocol to Build Locally Accurate Machine Learning Potentials. ***Journal of Chemical Information and Modeling***. *63(4)*, 1133-1142
12. Wang, Y., **Zhang, H**., Wang, J., Tang, G., & Bai, H. (2023). An Engineered Design of Self-Assembly Nanomedicine Guided by Molecular Dynamic Simulation for Photodynamic and Hypoxia-Directed Therapy. ***Molecular Pharmaceutics*** *20(4)*, 1543-8384.
13. Lin H, Yufei Huang, **Zhang, H.**, et al. DiffBP: Generative Diffusion of 3D Molecules for Target Protein Binding. Submitted to ***Journal of Medicinal Chemistry***. Code
14. Lin H, Yufei Huang, **Zhang, H.**, et al. Functional-Group-Based Diffusion for Pocket-Specific Molecule Generation and Elaboration. ***NeurIPS*** *2024.*
15. Du H.*, Jiang D.*, **Zhang, H.**, et al. A Flexible Data-Free Framework for Structure-Based De Novo Drug Design with Reinforcement Learning (2023). ***Chemical Science***. *14, 12166-12181*. Code
16. Chen H., **Zhang H.**, et al. (2023). Dynamics and kinetics of a long-flexible fatty acid binding with fatty acid binding protein. ***Journal of Chemical Informatics and Modeling***, *63, 16, 5232–5243.*
17. Zhao, Y., Zhang, J., **Zhang, H.**, Gu, S., Deng, Y., Tu, Y., ... & Kang, Y. (2023). Sigmoid Accelerated Molecular Dynamics: An Efficient Enhanced Sampling Method for Biosystems. *The Journal of Physical Chemistry Letters*, *14*(4), 1103-1112.
18. Jia, L., Feng, Z., **Zhang, H.**, Song, J., Zhong, Z., Yao, S., & Song, M. (2022). Explainable Fragment-Based Molecular Property Attribution. ***Advanced Intelligent Systems***, *4*(10), 2200104
19. Wang, T., …, **Zhang, H.**, …, Hou T., Comprehensive Assessment of Protein Loop Modeling Programs on Large-scale Datasets: Prediction Accuracy and Efficiency. Submitted to *Protein & Cell.*
20. Wang, S. P., Huang, X., He, Y., **Zhang, H.**, Zhou, J., Tang, G., ... & Bai, H. (2023). Amphiphilic porphyrin-based supramolecular self-assembly for photochemotherapy: From molecular design to application. ***Nano Today,*** *48*, 101732.

21. Yang Y., Chen G., **Zhang H.**, et al. Multi-Objective Structure-Based Molecule Generation with Pareto MCTS, *AAAI 2024, Submitted.*
22. Huang Y., Li S., Wu L., Su J., Lin H., **Zhang H**., Protein 3D Graph Structure Learning for Robust Structure-based Protein Property Prediction. *AAAI 2024.*
23. Jin, J., Wang, D., Shi, G., Bao, J., … **Zhang, H.**, …, Kang, Y., FFLOM: a flow-based autoregressive model for fragment-to-lead optimization. *Journal of Medicinal Chemistry. 66, 15*, 10808–10823. (2023) Code
24. Jiang, D., Ye, Z., Hsieh, C. Y., Yang, Z., Zhang, X., Kang, Y., ... & Hou, T. (2023). **MetalProGNet**: a structure-based deep graph model for metalloprotein–ligand interaction predictions. ***Chemical Science*** *14(8), 2054-2069.* Code
25. Jiang, D., Hui, Z., Hong, D., …, **Zhang, H.**, …, Hou, T. How Good Are Current Docking Programs at Nucleic acids-ligand Docking? a Comprehensive Evaluation. ***Journal of Chemical Theory and Computation***. *14(8),* 2054-2069 (2023). Code