ODIN ZHANG

(HAOTIAN ZHANG)

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EDUCATION

University of Washington — Seattle, U.S.
Ph.D. in Computer Science, Paul G. Allen School, advised by **David Baker** — 2024.9 –present

Zhejiang University — Hangzhou, China
M.S in Pharmaceutical science, advised by **Tingjun Hou** and **Changyu Hsieh** — 2022.9 –2024.6

- Baidu AI Scholarship (Top 10 Chinese Researchers Nationwide)
- Chu Kochen Scholarship. (Top 10 Graduate Student at ZJU)
- National Scholarship (Top 1 Graduate Student in Pharmacy Department)

Zhejiang University — Hangzhou, China
Dual B.S in Pharmaceutical science & Physics, advised by **Tingjun Hou** — 2018.9 –2022.6

- GPA: 3.85/4.00
- First Prize in China Undergraduate Physics Tournament (Top 0.1%)
- 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

Pledge Therapeutics — Greater Boston, U.S.
Structure-based AIDD consultant — 2024.03– 2024.09

- Applied the Gen-AI to two test cases (internal) and two test cases (External).
- Refined Gen-AI platform based on crystallographer, structural biologist, and medicinal chemist insight.
- Performed Lead optimization of a viral capsid targeting small molecule
- Performed Hit expansion against a viral protein based on existing fragment co-crystal structure data

Carbon Silicon AI — Hangzhou, China
Senior DL-Engineer, leading a 10-people group — 2022.05– 2024.03

- 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– 2022.05

- 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.

LEADERSHIP/TEAMWORK EXPERIENCE

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.

PUBLICATIONS

1. **Zhang, H.**, et al. ResGen is a pocket-aware 3D molecular generation model based on parallel multiscale modelling, ***Nature Machine Intelligence***, *5*, 1020–1030 (2023). Code
2. **Zhang, H.***, Tianyue Wang*, et al. Learning on topological surface and geometric structure for 3D molecular generation, ***Nature Computational Science***,3.10 (2023): 849-859. Code
3. **Zhang, H.*,** Jieyu Jin.*, ECloudGen: Access to Broader Chemical Space for Structure-based Molecule Generation. ***Nature Computational Science***, *first round review.*
4. Zhang, X.*, **Zhang, H.***, et al. Efficient and accurate large library ligand docking with KarmaDock. ***Nature Computational Science***, *3*, 739–740 (2023). Code
5. Chen, S., **Zhang, H.*,** et al. Deep lead optimization enveloped in protein pocket and its application in designing potent and selective ligands targeting LTK protein. ***Nature Machine Intelligence***, *2025.* Code
6. Wu, Z., **Zhang, H.**, Wang, X., et al. Leveraging Language Model for Advanced Multi-Property Molecular Optimization via Prompt Engineering. ***Nature Machine Intelligence***, 6, 1359-1369 (2024). Code
7. Zhao, H., **Zhang, H.**, Pushing the Boundaries of Protein-peptide Docking with Rational and Accurate Diffusion Generative Model. ***Nature Machine Intelligence,*** *second round review.* (通讯)
8. **Zhang, H.***, Huang, Y.*, Chen, S.*, et al. FragGen: towards 3D geometry reliable fragment-based molecular generation. ***Chemical Science*** 15.46 (2024): 19452-19465. Code
9. **Zhang, H.***, Lin, H*. et al, Deep Lead Optimization: Leveraging Generative AI for Structural Modification. ***Journal of the American Chemical Society*** 146.46 (2024): 31357-31370.
10. **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
11. Huang, Y.*, **Zhang, H**.*, Wu, L., Tan, C., Lin, H., Gao, Z., ... & Li, S. (2024). Re-Dock: Towards Flexible and Realistic Molecular Docking with Diffusion Bridge. ***ICML 2024***.
12. Lin, H.*, **Zhang, H.***, Zhao, H., Jiang, D., Wu, L., Liu, Z., ... & Li, S. Z. (2024). PPFlow: Target-aware Peptide Design with Torsional Flow Matching. ***ICML 2024***.
13. Wang, T.*, Zhang, X.*, **Zhang, H.***, et al. Highly accurate and efficient deep learning paradigm for full-atom protein loop modeling with KarmaLoop. ***Research*** *7 (2024): 0408*. Code
14. 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
15. Weng, G., **Zhao, H.**, Nie, D., Zhang, H., Liu, L., Hou, T., & Kang, Y. (2024). Rediscmol: Benchmarking molecular generation models in biological properties. ***Journal of Medicinal Chemistry,*** 67(2), 1533-1543.
16. 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.
17. Zhang, X., Shen, C., **Zhang, H.**, Kang, Y., Hsieh, C. Y., & Hou, T. (2024). Advancing Ligand Docking through Deep Learning: Challenges and Prospects in Virtual Screening. ***Accounts of Chemical Research***, 789-804.
18. Wang, M., Li, S., Wang, J., **Zhang., H**., et al. ClickGen: Directed Exploration of Synthesizable Chemical Space via Modular Reactions and Reinforcement Learning. ***Nature Communications***, *15(1), 10127.* Code
19. Lin H, Yufei Huang, **Zhang, H.**, et al. DiffBP: Generative Diffusion of 3D Molecules for Target Protein Binding. ***Chemical Science*** 16.3 (2025): 1417-1431.. Code
20. Lin H, Yufei Huang, **Zhang, H.**, et al. Functional-Group-Based Diffusion for Pocket-Specific Molecule Generation and Elaboration. ***NeurIPS 2024***, arxiv: 2306.13769.
21. Du H.*, Jiang D.*, **Zhang, H.**, et al. A Flexible Data-Free Framework for Structure-Based De Novo Drug Design with Reinforcement Learning. ***Chemical Science***, *14(43), 12166-12181.*. Code
22. 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.
23. 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