

MUJIE LIN

[Google Scholar Profile](#) (H-index: 9, Total Citations: 434) [Homepage](#)

(+86) 13710105245 ✦ mjlin25@stu.pku.edu.cn ✦ First-year Master Student

Research Interests: Artificial Intelligence-Driven Drug Discovery (AIDD) , LLM for Science, Computational Biology

EDUCATION

Master of Philosophy (M.Phil.) in Computer Science, Peking University 2025 - 2028

- GPA: 3.8/4.0
- **Core Courses:** Artificial Intelligence (A+), 3D Vision and Computational Photography (A+), Computer Graphics (A+)

Bachelor of Science (B.S.) in Biotechnology, South China University of Technology (985 project) 2021 - 2025

- Overall Rank: 1/56 CET4 587 CET6 527
- **Core Courses:** Genomics (92), Integrated Omics Data Analysis (98), Bioinformatics (90), Introduction to Synthetic Biology (91), Molecular Biology (90), Calculus (90), Probability Theory and Mathematical Statistics (90), Introduction to Mathematical Modeling (89), Molecular Biology Laboratory (100), etc.

Bachelor of Engineering (B.E.) in Computer Science (Minor), SCUT 2022 - 2025

- **Core Courses:** Discrete Mathematics, Advanced Programming, Data Structures, Python Programming, etc.

RESEARCH EXPERIENCE

MiniMax Co., Ltd. Beijing, China
LLM Algorithm Intern, Foundation Language Model Team Feb 2025 - Aug 2025

Center of Excellence on Generative AI, King Abdullah University of Science and Technology (KAUST)
Research Intern, Advisor: Wang Yu, Xin Gao Dec 2024 - Mar 2025

AI Computational Biology lab, Westlake University Hangzhou, China
Visiting Student, Advisor: Jianyang Zeng Jul 2024 - Aug 2024

DP Technology Co., Ltd. Beijing, China
AI4S Innovative Algorithm Researcher (Intern) , Mentor: Yongge Li Jul 2023 - Mar 2024

Artificial Intelligence and Medicinal Chemistry Laboratory, SCUT Guangzhou, China
Undergraduate Researcher, Advisor: Ling Wang Dec 2021 - Jul 2025

SELECTED PUBLICATIONS

Generative Modeling for Protein Dynamics & Efficient Inference

- **BioDynaSpec: Harmonic-Guided Spatio-Spectral Autoregressive Diffusion for Protein Dynamics Generation.** Mujie Lin, Yutian Liu, Yudi Guo, et al. *ICML 2026*. **First Author**. Proposed a spatio-spectral autoregressive diffusion framework for long-horizon protein dynamics generation, reducing trajectory error by over 60% against strong baselines.
- **Tikhonov-Stabilized Bézier Representation Forecasting for Training-free Diffusion Acceleration.** Lei Zhu[#], Mujie Lin[#], Ruochong Zheng, Guangyi Wang, Hao Li, Peng Jin, Chang Liu, Jie Chen. *NeurIPS 2026, under review*. **Co-first Author**. Developed BeziCast, a training-free diffusion acceleration method based on output-proximal representation forecasting, achieving up to $4.79\times$ speedup on image/video diffusion models.
- **ProAR: Probabilistic Autoregressive Modeling for Molecular Dynamics.** Kaiwen Cheng, Yutian Liu, Zhiwei Nie, Mujie Lin, et al. *AAAI 2026*. **Fourth Author**. Developed a probabilistic autoregressive framework for molecular dynamics generation with anti-drifting sampling and improved long-horizon trajectory consistency.

Scientific Foundation Models & LLM

- **MiniMax-M1: Scaling Test-Time Compute Efficiently with Lightning Attention.** Aili Chen, Aonian Li, et al., Mujie Lin, et al. *Technical Report*, 2025. **Contributor**. Contributed to automated evaluation infrastructure, science reasoning benchmarks, and model iteration analysis for MiniMax-M1.
- **SciAssess: Benchmarking LLM Proficiency in Scientific Literature Analysis.** Hengxing Cai[#], Xiaochen Cai[#], Junhan Chang[#], Sihang Li[#], et al., Mujie Lin, et al. *Findings of NAACL 2025*. Built scientific literature analysis benchmarks covering multimodal scientific understanding and reasoning tasks.
- **Uni-SMART: Universal Science Multimodal Analysis and Research Transformer.** Hengxing Cai, Xiaochen Cai, Shuwen Yang, et al., Mujie Lin, et al. *arXiv preprint*, 2024. Contributed to biological-domain evaluation tasks for multimodal scientific foundation models.

AI-driven Drug Discovery & Molecular Representation Learning

- **MalariaFlow: A Comprehensive Deep Learning Platform for Multistage Phenotypic Antimalarial Drug Discovery.** Mujie Lin, Junxi Cai, Yuancheng Wei, et al. *European Journal of Medicinal Chemistry*, 2024. **First Author**. Built a multistage antimalarial drug discovery benchmark and platform covering 10 phenotypes and 3 parasite lifecycle stages.
- **DeepCancerMap: A Versatile Deep Learning Platform for Target- and Cell-based Anticancer Drug Discovery.** Jingxing Wu[#], Yi Xiao[#], Mujie Lin[#], et al. *European Journal of Medicinal Chemistry*, 2023. **Co-first Author**. Constructed a large-scale anticancer drug discovery platform with target-based and cell-based virtual screening models.
- **FG-BERT: A Generalized and Self-supervised Functional Group-based Molecular Representation Learning Framework for Properties Prediction.** Biaoshun Li, Mujie Lin, Tiegeng Chen, Ling Wang. *Briefings in Bioinformatics*, 2023. **Second Author**. Proposed a functional-group-aware molecular pretraining framework for interpretable molecular property prediction.
- **Structure Prediction of Peptides Containing Non-canonical Amino Acids: A Comprehensive Benchmark of Full-Atom Algorithms.** Yu Wang[#], Yifan Deng[#], Fuming Zeng, Mujie Lin, et al. *Genomics, Proteomics & Bioinformatics*, 2026. **Fourth Author**. Benchmarked leading all-atom structure prediction models on canonical and chemically modified peptide-protein complexes.

ACADEMIC SERVICE

Invited Reviewer for International Journals

- *Scientific Reports* (Nature Portfolio, SCI JCR Q1, IF=4.03), 2025
- *Bioinformatics* (Oxford University Press, SCI JCR Q1, IF=5.4), 2025
- *Molecular Diversity* (Springer International Publishing, SCI JCR Q2, IF=3.9), 2025

Invited Reviewer for International Conferences

- *ACM MM 2026* (34th ACM International Conference on Multimedia), 2026
- *NeurIPS 2026* (The Fortieth Annual Conference on Neural Information Processing Systems), 2026

AWARDS AND HONORS

Chinese National Scholarship for the 2022-2023 Academic Year

”Chinese University Students’ Self-reliance Star” Scholarship Nominated

The 18th ”Challenge Cup” National Undergraduate Extracurricular Academic Science and Technology Competition, *Jointly Responsible* Grand Prize (Top 0.01%)

National College Student Innovation Training Program, *Project Leader* Outstanding Completion

The 9th China International College Students Innovation Competition (Guangdong) Bronze Prize

’Huashu Cup’ International Mathematical Contest in Modeling 2023, *Leader* Honorable Mention

Asia and Pacific Mathematical Contest in Modeling Certificate of Achievement 2022 Third Prize

National Undergraduate Mathematical Contest in Modeling (Guangdong), *Leader* Third Prize

Contribution Award for Student Extracurricular Academic and Scientific Innovation Outstanding, 2023

Contribution Award for Student Extracurricular Academic and Scientific Innovation Excellent, 2022