

Yiyan Liao

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Peking University, 5 Yiheyuan Road, Haidian District, Beijing, 100871, China

EDUCATION

School of Life Sciences, Peking University (Top 1 Univ. in China, QS #14) Sept. 2023 - Present

- Major: Bioinformatics; Degree: Bachelor of Engineering
- Comprehensive Assessment Ranking (Entire Grade): 7/134 (Aug. 2025)

RESEARCH EXPERIENCES

Molecular Design Laboratory (MDL) at Peking University

Research: Computer-Aided Molecular Glue Discovery and Design Sept. 2024 - Present

- Under the supervision of **Dr. Jianfeng Pei** and **Prof. Luhua Lai**, Center for Quantitative Biology, Academy for Advanced Interdisciplinary Studies, Peking University.
- Systematically collected molecular glue data from various publications and curated the **The MGTbind (Molecular Glue and Ternary binding) database** (Co-first author, *Nucleic Acids Research Database Issue*).
- Evaluated the capacity of **AlphaFold 3** series models for predicting **molecular glue ternary complex structures** by constructing **MGBench** (Co-first author, *Journal of Chemical Information and Modeling*).
- Constructed a **diffusion-based docking method** to model molecular glue ternary **complex structures** (ongoing), and developed a **MD-based scoring model** for molecular glue ternary **binding affinities** (ongoing).

Data Structure Lab (DS-Lab) at Peking University

Intern: Reinforcement Learning Intern at Moonshot AI Jan. 2025 – Jun. 2025

- Enhancing **Large Language Model (LLM)** capabilities in the **biology domain** through **reinforcement learning**, specifically targeting improved performance on the **Graduate-Level Google-Proof Q&A (GPQA)** Benchmark.

Intern: Biological Large Language Model Intern at Tencent Jun. 2025 – Present

- Training **biological reasoning LLMs** and **foundation LLMs**.

Research: Scientific Benchmarks Construction Jan. 2025 – Present

- Under the supervision of **Dr. Tong Yang**, Associate Professor, School of Computer Science, Peking University.
- Contributed to the development of several LLM benchmarks: **SuperGPQA** (graduate-level knowledge; Core contributor, *NeurIPS 2025*), **SciDA** (dynamic scientific benchmark; Third author, under review by *ICLR 2026*), and **ScholarSearch** (academic information retrieval; Co-first author, under review by *AAAI 2026*).

International Genetically Engineered Machine (iGEM)

Wet Lab Leader: Team Peking 2024 Jan. 2024 – Oct. 2024

- Led the experimental design and implementation for the project, "**General disease detection with Protease and Aptamer**".
- Awarded the **Gold Medal** at the 2024 iGEM Grand Jamboree.

Advisor: Team Peking 2025 Jan. 2025 – Present

- Participated in selecting members for **Team Peking 2025** and provided research advice for their projects.

RESEARCH INTERESTS

- Computer-aided molecular glue (MG) discovery
- Structural geometry deep learning & modeling
- Reasoning & foundation biological large language models (LLMs)

PUBLICATIONS

- **MGTbind: a comprehensive database of molecular glue ternary interactome**
Jintao Zhu*, **Yiyan Liao***, Haoyu Lin*, ..., Luhua Lai, Jianfeng Pei
Nucleic Acids Research, 2025. <https://doi.org/10.1093/nar/gkaf1075>
- **Benchmarking Cofolding Methods for Molecular Glue Ternary Structure Prediction**
Yiyan Liao*, Jintao Zhu*, Juan Xie, Luhua Lai, Jianfeng Pei
Journal of Chemical Information and Modeling, 2025. <https://doi.org/10.1021/acs.jcim.5c01860>
- **ScholarSearch: Benchmarking Scholar Searching Ability of LLMs**
Junting Zhou*, Wang Li*, **Yiyan Liao***, ..., Yuhan Wu, Tong Yang
In review, 2025. <https://doi.org/10.48550/arXiv.2506.13784>
- **SciDA: Scientific Dynamic Assessor of LLMs**
Junting Zhou*, Tingjia Miao*, **Yiyan Liao**, ..., Yitao Liang, Tong Yang, Wenhao Huang, Ge Zhang
In review, 2025. <https://doi.org/10.48550/arXiv.2506.12909>
- **SuperGPQA: Scaling LLM Evaluation across 285 Graduate Disciplines**
M-A-P Team, Xinrun Du, Yifan Yao, ..., **Yiyan Liao**, ..., Jiaheng Liu, Qunshu Lin, Wenhao Huang, Ge Zhang
NeurIPS, 2025. <https://doi.org/10.48550/arXiv.2502.14739>

ACADEMIC ACHIEVEMENTS

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|---|------------|
| 2024-2025 Peking University Merit Student | Sept. 2025 |
| • Top ~14% of entire grade | |
| 2024-2025 Peking University Qin Wanshun Jin Yunhui Scholarship | Sept. 2025 |
| • Total ~150 for students at Peking University | |
| 2025 Beijing Natural Science Foundation Undergraduate Research Program | Jul. 2025 |
| • Development and Validation of Deep Learning-Based Virtual Screening Methods for Molecular Glues | |
| 33th Peking University “Challenge Cup” Competition | May. 2025 |
| • Excellence award (team leader) | |
| International Genetically Engineered Machine (iGEM) 2024 | Oct. 2024 |
| • Gold medal for team Peking, as wet lab leader | |
| MingDe Scholarship | Dec. 2023 |
| • Peking University first prize scholarship for freshmen (~50 students) | |
| 34th International Biology Olympiad (IBO) | Jul. 2023 |
| • Gold medal (third place) | |
| 31st China National Biology Olympiad (CNBO) | Aug. 2022 |
| • Gold medal (national team member) | |

SKILLS

- **Programming:** Python, R, MATLAB, Linux, High-Performance Computing (HPC) clusters
- **Software:** Schrödinger, PyMOL, ChimeraX
- **Large Language Models:** LLaMA Factory, Supervised Fine-Tuning (SFT), Reinforcement Learning (RL)
- **Experimental Skills:** Molecular cloning, Surface Plasmon Resonance (SPR), Western Blot (WB), etc.
- **Languages:** Chinese (First), English (TOEFL: 103/120)

SELECTED COURSES

- Linux-based Essential Bioinformatics(LEB) (A/A)
- Innovative Experiments in Bioinformatics (A/A)
- Bioinformatics (A/A)
- Artificial Intelligence for Protein Design (94/100)