

JunLin Yu



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Education

SiChuan University



Chengdu, China

Ph.D. in Pharmacy, West China School of Pharmacy

2023.9 - present

My research focus on geometric deep learning and knowledge-guided intelligent system for drug design and drug discovery.

M.S. in Pharmacy, West China School of Pharmacy

2020.9 - 2023.6

My research focus on metalloenzyme data and analysis, including traditional and deep learning-based metal-binding site identification algorithm, metalloenzyme data mining and curation, metalloenzyme-centric score function design.

B.A. in Pharmacy, West China School of Pharmacy

2016.9 - 2020.6

Research interests

Geometric Deep Learning, Generative Model; Knowledge Guidance; Biochemistry

Honors & Awards

Doctoral Fellowship in Youth Science and

2026-2027 **Technology Talent Program**, China Association for
Science and Technology

Chengdu, China

2026-2027 **Student membership**, CAAI

Chengdu, China

2025 **National Scholarship**, SiChuan University

Chengdu, China

2025 **Best Poster 1st Class**, AHeDD, ZheJiang University

Hangzhou, China

2025 **Oral presentation**, ACS Spring 2025

San Diego, US

2023 **Second Prize**, "Internet +" College Student Innovation
and Entrepreneurship Competition

Chengdu, China

2023 **Outstanding Presentation Award**, National
Academic Symposium for Pharmacy Graduate
Students

Shenyang, China

2017 **National Encouragement Scholarship**, SiChuan
University

Chengdu, China

Publications

1. **Yu, J.-L.**; et al. Knowledge-Guided Diffusion Model for 3D Ligand-Pharmacophore Mapping. *Nat. Commun.* 2025, 16, 2269.
2. Peng, J.*; **Yu, J.-L.***; et, al. Pharmacophore-Oriented 3D Molecular Generation towards Efficient Feature-Customized Drug Discovery. *Nat. Comput. Sci.*, 2025.
3. **Yu, J.-L.**; et al. MeDBA: the Metalloenzyme Data Bank and Analysis platform. *Nucleic Acids Research* 2023, 51, D593-D602.
4. Zhang Y.-D.; **Yu, J.-L.**, et al. REaMA: Building Biomedical Relation Extraction Specialized Large Language Models Through Instruction Tuning. *IEEE Trans. Neural Networks Learn. Syst.*, 2025.
5. **Yu, J.-L.**; et al. Geometric deep learning-enabled metal-binding site identification and grafting. *Fundamental Research* 2024.
6. Wu J.-W.; Ning X.-L.; Tang B.-D.; Chen Y.-T.; Yang Z.-B.; Meng F.-B.; Zhou C.; **Yu J.-L.**; et al. Deciphering Glutaminyl Cyclase Catalytic Pathways Enables Recognition of Anchor Pharmacophores for Discovering New Inhibitors. *J. Chem. Inform. Model.* 2025, 65, 5006–5018.
7. Zhou, C.; Cai, C.-P.; Huang, X.-T.; **Yu, J.-L.**; et al. TarKG: A Comprehensive Biomedical Knowledge Graph for Target Discovery. *Bioinformatics* 2024, 40.
8. **Yu, J.-L.**; et al. Advances in Computer-aided Metalloenzyme-targeted Drug Discovery. *Chinese Journal of Modern Applied Pharmacy* 2022, 39, 2828-2833.
9. **Yu, J.-L.**; et al. Deep learning in target prediction and drug repositioning: recent advances and challenges. *Drug Discovery Today* 2022.
10. Dai, Q.-Q.*; **Yu, J.-L.***; et al. Recent Advances in Deep Learning Aided Drug Discovery. *Progress in Pharmaceutical Sciences* 2022, 46, 60-70.
11. Yan, Y.-H.; Li, Z.-F.; Ning, X.-L.; Deng, J.; **Yu, J.-L.**; et al. Discovery of 3-Aryl Substituted Benzoxaboroles as Broad-Spectrum Inhibitors of Serine- and Metallo- β -Lactamases. *Bioorg. Med. Chem. Lett.* 2021, 41, 127956.
12. Xiao, Y.-C. ; **Yu, J.-L.**; et al. Targeting Metalloenzymes by Boron-Containing Metal-Binding Pharmacophores. *J. Med. Chem.* 2021, 64, 17706-17727.
13. Xiao, Y.-C.; Chen, X.-P.; Deng, J.; Yan, Y.-H.; Zhu, K.-R.; Li, G.; **Yu, J.-L.**; et al. Design and enantioselective synthesis of 3-(α -acrylic acid) benzoxaboroles to combat carbapenemase resistance. *Chem. Commun.* 2021, 57, 7709-7712.
14. Ning, X.-L.; Li, Y.-Z.; Huo, C.; Deng, J.; Gao, C.; Zhu, K.-R.; Wang, M.; Wu, Y.-X.; **Yu, J.-L.**; et al. X-ray Structure-Guided Discovery of a Potent, Orally Bioavailable, Dual Human Indoleamine/Tryptophan 2,3-Dioxygenase (hIDO/hTDO) Inhibitor That Shows Activity in a Mouse Model of Parkinson's Disease. *J. Med. Chem.* 2021, 64, 8303-8332.