

# JunLin Yu

West China School of Pharmacy  
SiChuan University, Chengdu, China

+86 13208186198 | Email: [yujunlin@stu.scu.edu.cn](mailto:yujunlin@stu.scu.edu.cn) | [ORCID](#) | [Github](#)



## Education

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### 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

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Geometric Deep Learning, Generative Model; Knowledge Guidance; Biochemistry

## Honors & Awards

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2026-2027	<b>Doctoral Fellowship in Youth Science and Technology Talent Program</b> , China Association for Science and Technology	Chengdu, China
2026-2027	<b>Student membership</b> , CAAI	Chengdu, China
2025	<b>National Scholarship</b> , SiChuan University	Chengdu, China
2025	<b>Best Poster 1st Class</b> , AHeDD, ZheJiang University	Hangzhou, China
2025	<b>Oral presentation</b> , ACS Spring 2025	San Diego, US
2023	<b>Second Prize</b> , "Internet +" College Student Innovation and Entrepreneurship Competition	Chengdu, China
2023	<b>Outstanding Presentation Award</b> , National Academic Symposium for Pharmacy Graduate Students	Shenyang, China
2017	<b>National Encouragement Scholarship</b> , SiChuan University	Chengdu, China

## Publications

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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- $\beta$ -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-( $\alpha$ -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.