

Yuquan Xu

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Research Interests

AI for drug discovery; AI for precision medicine; drug combination prediction; drug repurposing

Research Profile

My research focuses on developing AI methods for drug discovery and precision medicine, particularly graph-based and multimodal approaches for modeling relationships among drugs, genes, diseases, and cellular contexts. Building on a research background in biomedical image analysis, I now focus on drug combination prediction, drug repurposing, and interpretable therapeutic discovery.

Education

Yong Loo Lin School of Medicine, National University of Singapore	Singapore
Master of Science in Precision Health and Medicine	2025–2027 (Expected)
Grade: 4.3/5.0	
Stirling College, Chengdu University (Sino-Foreign Cooperation Program)	Chengdu, China
Bachelor of Science with Honours in Data Science (University of Stirling)	2021–2025
Grade: 77.64% (First Class), Rank: 1/99	
Bachelor of Engineering in Data Science (Chengdu University)	
Grade: 85.83%, Rank: 3/99	

Publications and Manuscripts

Submitted Manuscripts

- Y. Xu, Y. Zhang, Y. Wan, Y. Yang, C. Xie, J. Song, and Y. Wang. Decoupling Multi-Granularity Perception and Harmonizing Inductive Biases for Robust Medical Image Segmentation. Submitted to *Engineering Applications of Artificial Intelligence*.
- Y. Wan, Z. Chen, Y. Xu, M. Li, and Y. Wang. Breaking Error Coupling via Divergent-Convergent Coordination for Semi-Supervised Medical Image Segmentation. Submitted to *Medical Image Analysis*.

Peer-Reviewed Publications

- Y. Xu, T. M. Rajeh, Y. Zhang, L. Zhang, Y. Wan, J. Joo, and Y. Wang. Enhancing Cross-Dataset Generalization with Quasi-Multimodal Training and the Diamond Hybrid Backbone. *Biomedical Signal Processing and Control*, 2026.
- X. Wang, Y. Wang, Y. Xu, Y. Zhang, and L. Zhang. MMTU-Net: Enhancing Medical Image Semantic Segmentation with Multi-level Multi-scale Fusion and Transformer. *The Visual Computer*, 2025.
- Y. Wang, Y. Zhang, L. Zhang, Y. Wan, Z. Chen, Y. Xu, R. Cao, L. Zhao, Y. Yang, and X. Yu. A feature enhancement network based on image partitioning in a multi-branch encoder-decoder architecture. *Knowledge-Based Systems*, 2025.
- R. Feng, Y. Wang, J. Xue, Y. Xu, and X. Yu. CLAC-Net: Enhanced Detail Segmentation Framework Based on Self-Attention with Cross-Layer Fusion and Asymmetric Connections. *The Visual Computer*, 2024.

- Y. Wang, **Y. Xu**, X. Yu, and R. Feng. Flattened and simplified SSCU-Net: exploring the convolution potential for medical image segmentation. *The Journal of Supercomputing*, 2024.
- Y. Wang, Y. Zhang, L. Zhang, **Y. Xu**, R. Feng, H. Song, H. Cai, Z. Zhao, J. Xue, Z. Wang, S. Qiu, Y. Yang, and X. Yu. Multi-Bottleneck progressive propulsion network for medical image semantic segmentation with integrated macro-micro dual-stage feature enhancement and refinement. *Expert Systems With Applications*, 2024.
- Y. Wang, X. Yu, Y. Yang, S. Zeng, **Y. Xu**, and R. Feng. FTUNet: A Feature-Enhanced Network for Medical Image Segmentation Based on the Combination of U-Shaped Network and Vision Transformer. *Neural Processing Letters*, 2024.

Research Experience

Hypergraph Learning for Drug Combination Prediction

MBZUAI

Advisor: Prof. Jun Wen

2025–Present

- Developing hypergraph models for drug combination prediction using multimodal biomedical data.
- Building a knowledge graph to model drug–cell line relationships.
- Improving model interpretability through biologically informed design.

ML-guided Discovery of GBA1 Pharmacological Chaperones

National University of Singapore

Advisor: Dr. Xavier Chee Wezen

2026–Present

- Developing a machine learning workflow to identify candidate pharmacological chaperones for GBA1.
- Curating ligand data for allosteric binding prediction.
- Investigating binding mechanisms using QSAR and molecular dynamics.

Topology-aware Modeling for GWAS

National University of Singapore

Advisor: Prof. Caroline Lee

2025–Present

- Exploring a dual-view framework that combines graph neural networks and vision transformers for GWAS tasks.
- Investigating few-shot and self-supervised learning for genomic modeling.
- Benchmarking the framework against polygenic risk score baselines.

Medical Image Segmentation

Chengdu University

Advisor: Prof. Yuefei Wang

2022–2026

- Built and curated a 210k+ medical image dataset for model development and benchmarking.
- Contributed to segmentation model design, leading to multiple journal publications.
- Improved experimental efficiency through reusable research workflows and engineering scripts.

Technical Skills

Programming: Python, R, Java

Frameworks and Libraries: PyTorch, TensorFlow

Data and Databases: MySQL, MongoDB

Research Tools: OriginLab

Honors and Scholarships

Outstanding Graduation Thesis, Chengdu University	2025
Outstanding Graduate of Sichuan Province	2024
Outstanding Graduate of Chengdu University	2024
Special Prize Scholarship (Top 1%)	2022
First Prize Scholarship (Top 3%)	2023, 2024

Additional Experience

Software Development Engineer (Intern), CASCO 2025

Developed backend APIs and data-driven modules for a national railway system.

Data Analyst (Intern), Wanyi Devices Group 2024

Automated reporting workflows in Python and supported equipment utilization analysis.