Xiang Zhang

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EDUCATION

Shanghai Institute of Materia Medica & **NJUCM**   Sept. 2021 - Jul. 2025
M.Pharm. in Drug Design, GPA: 3.8/4
Advisor: Prof. Dr. Mingyue Zheng and Dr. Xutong Li

Henan University   Sept. 2017 - Jul. 2021
B.S. in Pharmaceutics, GPA: 3.3/4

WORK EXPERIENCE

Hengqin Lab, GMTCM   Sept. 2025 - present
Research Assistant, lead by Prof. Dr. Yong Liang and Prof. Dr. Xiaojun Yao
– Developing a Agent+MCP based Molecule Generation Model. (SCI Q2 expected)
– Writing a review about AI-assisted Medicinal Chemistry. (in revise, SCI Q1 expected)

RESEARCH INTEREST

AI for Medicinal Chemistry: Retrosynthesis & Synthesizability Prediction, Molecule Generation.
Agent: LLM Coordinator Design, MCP/API Engineering, Online Tool Deployment.

RESEARCH EXPERIENCE

Synthetic Accessibility Prediction   Jul. 2023 - Feb. 2025
– Developed SynFrag, a fragment assembly auto-regressive generation model for SA prediction, desired by simulating the stepwise assembly of building blocks in synthesis.
– Curated 9.2M pre-training and 800k fine-tuning dataset, contributing two application scenario test sets. SynFrag achieved SOTA while demonstrating chemical interpretability.
– Deployed SynFrag online service: sub-second & interpretable prediction.   [Web]

Molecular Property Prediction   Oct. 2024 - Jun. 2025
– Develop BioCLIP, a progressive multi-modal bootstrapping framework that address the scarcity of tri-modal data through hierarchical training, for diverse molecular property predictions. [Code]

Organic Synthesis   Jan. 2022 - Sept. 2022
– Synthesis, Purification, and Analysis of PROTAC Intermediates in Prof. Dr. Chen's Lab.

PUBLICATIONS

[1] **Zhang, X.**, Liu, J., Chen, K. (Academician). SynFrag: Synthetic Accessibility Predictor based on Fragment Assembly Generation in Drug Discovery. *JCIM*, 2025.   [DOI] | [Code] | [PDF]

[2] Fan, Z., Yu, J., **Zhang, X**. Reducing overconfident errors in molecular property classification using Posterior Network. *Patterns*, 2024, **5**(6):100991.   [DOI] | [Code] | [PDF]

SKILLS

· Programming/Software: Python, Pytorch, HTML, LaTeX, Flask, Prism, ChemDraw, PyMOL
· Cheminformatics: RDkit, DGL, deepchem, GNN, Transformer, RL, Contrastive Learning
· in Laboratory: Organic synthesis, purification & analysis
· Language: English (fluent, CET6: 520), Chinese (native), Cantonese (native), Hakka (native)

CONFERENCE

· Oral Presentation: The 13th Shanghai Symposium on Computer-Aided Drug Design | 2024
· Participation: World Artificial Intelligence Conference (WAIC), Shanghai | 2022, 2023, 2025

AWARDS & HONORS

· Academic Excellence Scholarship | 2021 - 2024
· Certificate of Honor for volunteer in COVID-19 Prevention | 2022