

XIANG ZHANG

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EDUCATION

Shanghai Institute of Materia Medica, CAS & NJUCM

Shanghai, China

- Master of Medicine in AI aided Drug Design, (GPA: 3.8/4) Sep.2021 - Jun.2025
- Supervisor: Prof. [Mingyue Zheng](#) (Google Scholar)
- Thesis: Molecular Synthetic Accessibility Prediction Model Based on Fragment Assembly auto-Regressive Pretrain and Related Model Evaluations. (Recommended as Outstanding Master's Thesis (top 10%))

Henan University

Kaifeng, China

- Bachelor of Science in Pharmacy Sep.2017 - Jun.2021

RESEARCH EXPERIENCE

Deep Learning-Based Prediction of Molecular Synthetic Accessibility

Oct.2023 - May.2025

- Designed FARScore with fragment assembly autoregressive pretraining to simulate molecular construction, fine-tuned for synthetic accessibility prediction.
- Curated 9.2M pretraining molecules (ChEMBL/ZINC...) and 800k labeled molecules (50% easy/50% hard synthesis) for model fine-tuning, optimizing hyperparameters via random search & early stopping.
- Achieved SOTA on three public benchmarks and built two specialized test sets (AI-generated molecules & clinical candidates) where FARScore outperformed 7 models.
- Conducted interpretability experiments: ablation studies, assembly path visualization, rare fragment impact analysis, and atomic attention mapping.

PUBLICATIONS

- **Zhang X**, Liu J, Li X, et al. FARScore: A Synthetic Accessibility Predictor based on Fragment Assembly autoRegressive Pretrain, *Journal of Cheminformatics*, (Submitted). [Github](#)
- Fan Z, Yu J, **Zhang X**, et al. Reducing overconfident errors in molecular property classification using Posterior Network[J]. *Patterns*, 2024, 5(6). DOI: <https://doi.org/10.1016/j.patter.2024.100991>

TECHNICAL EXPERTICE

- **ML/DL**: Python, Pytorch, Scikit-learn, GNNs, GANs, Transformer, DGL, TensorBoard, Matplotlib
- **Cheminformatics**: RDkit, DeepChem, Schrödinger Suite, PyMOL, ChemDraw
- **Medicinal Chemistry**: Multi-step organic synthesis, Purification, LC-MS

CONFERENCE

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

AWARDS & HONORS

- Academic Excellence Scholarship (3 consecutive years) | 2022-2024
- Certificate of COVID-19 Prevention Volunteer | 2022

LANGUAGES

- Chinese: Cantonese (native), Mandarin (native), Hakka (native).
- English: Professional Working Proficiency. (IELTS: 7.0 anticipated)