Yijingxiu (Louise) Lu





EDUCATION

Seoul National University

Computer Science, Master and Ph.D.

Sep. 2018 - Dec. 2025 Seoul, South Korea

o GPA: 3.83/4.20

University of Science and Technology Beijing

Iune. 2017

Communication Engineering, Bachelor

Beijing, China

o GPA: 3.34/4.00

· Hefei NO.6 High School

June. 2013

Science, Secondary Education

Hefei, China

• Grade: 1.5%

LANGUAGES

- English: Business and Academic Proficiency
- Korean: Business Proficiency
- Chineses: Native

SKILLS

- Programming Languages: Python, C++, MATLAB, LaTeX
- Data Science & Machine Learning: PyTorch, TensorFlow, HuggingFace, PyG, TorchDrug, RDKit, Matplotlib
- Research Tools: AutoDock Vina, ChemDraw, PyMOL, Cytoscape
- Web Technologies: HTML, CSS, JavaScript, Django, D3.js, 3Dmol.js, Bootstrap
- Database Systems: SQL
- Research Skills: Experimental Design, Data Analysis, Literature Review, Interdisciplinary Collaboration

HONORS AND AWARDS

Excellent Poster Award

Oct. 2024

BIOINFO/2024 Annual Conference of Korean Society for Bioinformatics

Presented paper: "Condition Aware Relational Learning for Chemical Reaction Yields Prediction"

Notable Paper Award

May. 2024

Second ICLR Tiny Paper Track/ICLR

Presented paper: "Enhancing Drug-Drug Interaction Prediction with Context-Aware Architecture"

Samsung HumanTech Paper Award

Feb. 2024

Samsung Advanced Institute of Technology/Samsung

 Presented paper "Improving Out-of-Distribution Generalization in Graphs with Hierarchical Semantic Environments" (co-author)

• Excellent Project Award

Dec. 2022

"Chunhui Cup" Oversea Students Innovation and Entrepreneurship Competition, Ministry of Education, PRC

Lead project: "Artificial Intelligence-Based COVID-19 Target Discovery and Drug Design"

· Global AI & Big Data Scholarship

Jan. 2021 - Jan. 2022

Daewoong Foundation

 Project focus: Improving drug-likeness of generated molecules using designed objective functions and a VAE framework

Global Scholarship II

Mar. 2019 - Jun. 2021

Office of International Affairs/Seoul National University

1st Prize in Computer Games

Aug. 2016

National Computer Games Tournament, China

Awarded in categories "EinStein würfelt nicht!" and "Dots and Boxes"

1st Prize in Software Design and Development Competition

Jul. 2014

Computer and Communication Engineering School, USTB

LEADERSHIP EXPERIENCE

Head Teaching Assistant

Seoul National University

Seoul National University, Department of Computer Science

Sep. 2024 - Dec. 2024

• Led the 2024-2 Algorithm (001) course, coordinating teaching assistant activities and mentoring team members.

Head Student, Bio & Health Informatics Lab

Aug. 2023 - Aug. 2024

[)

· Managed academic and administrative affairs, organized lab meetings, and oversaw intern management.

• Teaching Assistant, Machine Learning in Bioinformatics (001)

Mar. 2024 - Jun. 2024

Seoul National University, Department of Computer Science

• Delivered lectures on deep learning methodologies and their applications on bioinformatics.

• Teaching Assistant, AI-BIO

Sep. 2022 - Dec. 2022

Seoul National University, Artificial Intelligence Institute

Delivered lectures on AI-based drug discovery (drug-target interaction prediction models).

• Implement Deep Learning Model on Self-Built Website

Aug. 2022

[#]

Bio & Health Informatics Lab/Seoul National University

c.

 \circ Implemented our proposed drug-target interaction prediction model and diffdock on our website.

• Lab Website Maintain

Aug. 2020 - Aug. 2023

Bio & Health Informatics Lab/Seoul National University

• Maintain the homepage of BHI lab.

Aug. 2020 - Aug. 2023

PATENTS AND PUBLICATIONS

C=Conference, J=Journal, P=Patent, W=Workshop, S=In Submission

[S.2] Lu Y., Piao Y., & Kim S. (2025). Reaction Yield Prediction with Chemical Role Aware Learning.

[W.2] [S.1] Lu Y., Lee S., Kang S., & Kim S. (2025). Mixture-of-Experts Approach for Enhanced Drug-Target Interaction Prediction and Confidence Assessment. Accepted at BIOKDD 2024. Invited submission for publication in IEEE ACM TCBB.

[J.2] [W.1] Lu Y., Piao Y., Lee S., & Kim S. (2025). Context-Aware Hierarchical Fusion for Drug Relational Learning. Accepted at BIOKDD 2024. *IEEE Transactions on Computational Biology and Bioinformatics* (2025).

[C.3] Piao Y., Lee S., Lu Y., Kim S. (2024). Improving out-of-distribution generalization in graphs via hierarchical semantic environments. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*.

[C.2] Lu Y., Piao Y., & Kim S. (2024). Enhancing Drug-Drug Interaction Prediction with Context-Aware Architecture. In *The Second Tiny Papers Track at ICLR* 2024.

[C.1] Choi MG., Shin W., Lu Y., & Kim S. (2023). Triangular Contrastive Learning on Molecular Graphs. In *Molecular Machine Learning Conference (MOML 2023)*.

[P.1] Lim S., Kim S., Lu Y., et al. (2022). Device and Method for Predicting Interactions Between Compounds and Proteins. Assigned to Seoul National University, Patent No. 0534-20210052.

[J.1] Lim S.*, Lu Y.*, Cho C Y., et al. (2021). A review on compound-protein interaction prediction methods: data, format, representation and model. Computational and Structural Biotechnology Journal.