Yijingxiu (Louise) Lu

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Education

- **Seoul National University** *Sep. 2018 - Dec. 2025*
  Computer Science, Master and Ph.D. Seoul, South Korea
  ◦ GPA: 3.83/4.20

- **University of Science and Technology Beijing** *June. 2017*
  Communication Engineering, Bachelor Beijing, China
  ◦ 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, Schröinger, Stardrop, 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

- **Outstanding Self-financed Student** *Jun. 2025*
  The Chinese Government Award for Outstanding Self-financed Students Abroad
- **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

- **Teaching Assistant, ML-Bio** *Mar. 2025 - Jun. 2025*
  Seoul National University, Department of Computer Science
  ◦ Delivered lectures on Artificial Intelligence Technologies and Appilications on Bioinformatics.
- **Head Teaching Assistant** *Sep. 2024 - Dec. 2024*
  Seoul National University, Department of Computer Science
  ◦ 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*
  Seoul National University [🌐]
  ◦ 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 [🌐]
  ◦ 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.

Patents and Publications

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

[J.3] **Lu Y.**, Piao Y., Shen M., & Kim S. (2025). **Improving Reaction Yield Prediction with Chemical Atom-Level Reaction Learning**. *Journal of Chemical Information and Modeling* (2025).

[C.4] Southiratn T., Koo B., **Lu Y.**, Kim S. (2025). **CombiMOTS: Combinatorial Multi-Objective Tree Search For Dual-Target Molecule Generation**. In *Forty-second International Conference on Machine Learning (ICML)*.

[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, Notable, Oral Presentation*.

[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, SNU-2022-06253.

[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*.

Academic Services

KDD 2025 Research Track Excellent Reviewer.
KDD 2024 Research Track Commendable Reviewer.
AAAI Reviewer (from 2023)

Other Activities

BOE 2025 Overseas Campus Ambassador (Seoul National University, Republic of Korea)
SNU 2020 SHANUM Multicultural Society for Social Responsibility Mentor