

Chan Young Joe

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CURRENT POSITION

Researcher, Data Science Team

Research Institute of Environmental Health and Safety, EH R&C Co.

Jan. 2026 – Present

Incheon, Korea

EDUCATION

University of Seoul

M.S. in Applied Chemistry (Computational Chemistry), advisor Prof. Rakwoo Chang

Seoul, Korea

Sep. 2024 – Feb. 2026

University of Seoul

B.S. in Applied Chemistry; B.E. in Artificial Intelligence (double major)

Seoul, Korea

Mar. 2021 – Aug. 2024

National Institute for Lifelong Education (NILE), Korea University

B.S. in Mathematics

Seoul, Korea

Jan. 2025 – Dec. 2026 (expected)

RESEARCH EXPERIENCE

Researcher, Computational Molecular Modeling Laboratory

University of Seoul (Prof. Rakwoo Chang)

Jun. 2021 – Feb. 2026

Seoul, Korea

- Large language models (in-context learning, fine-tuning) for molecular property prediction
- Molecular dynamics of membranes and enzymes; hybrid multigrained sampling

Visiting Researcher, Department of Bioengineering

Lehigh University (Prof. Wonpil Im)

Jun. 2024 – Aug. 2024

Bethlehem, PA, USA

SELECTED PUBLICATIONS

Lee, J.-H.*; **Joe, C. Y.** A flux-based bioaccumulation model for growing organisms: integrating advective–diffusive uptake at exchange organs into dynamic energy budget theory. *Environ. Toxicol. Chem.* **2026**, vgap253, DOI: 10.1093/etjnl/vgap253.

Joe, C. Y.; Song, K.*; Chang, R.* Evaluating in-context learning in large language models for molecular property regression. *J. Comput. Chem.* **2026**, 47, e70308, DOI: 10.1002/jcc.70308.

OPEN-SOURCE SOFTWARE

PFAS–rice uptake model | Python, HYDRUS-1D, Streamlit

github.com/ccy5123/pfas-rice-model

- Mechanistic four-compartment (root–stem–leaf–grain) uptake model for anionic PFAS in paddy rice, covering 12 calibrated PFCA/PFSA congeners
- Coupled to HYDRUS-1D soil transport; parameterisable from chemical structure; interactive web application

sci-adk | Python, Claude Code

github.com/ccy5123/sci-adk

- Verification kit for agent-assisted research: AI agents propose, and a deterministic engine judges each claim against decision rules frozen before the experiment
- Append-only evidence record with headless re-verification by third parties and tamper-evident provenance

SELECTED PRESENTATIONS

Joe, C. Y.; Lee, J.-H.* Integrated DEB-TK model for fish bioaccumulation assessment of neutral organic chemicals: theoretical formulation and empirical validation. Presented at the 2026 Spring General Meeting of the Korean Society of Environmental Health, Jeju, Korea, May 2026; poster P-EaRA-40. Best Poster Award.

Joe, C. Y.; Song, K.*; Chang, R.* Evaluating in-context learning in large language models for molecular property regression. Presented at Pacificchem 2025, Honolulu, HI, Dec. 15–20, 2025; poster PHY006.

*Corresponding author

HONORS

Best Poster Award, 2026 Spring General Meeting of the Korean Society of Environmental Health	2026
Outstanding Paper Award, President of the University of Seoul (<i>J. Comput. Chem.</i> paper)	2026
Best Poster Award, System Chemistry Global Leading Research Center Winter Symposium	2025
Best Poster Award, Fall Meeting of the Korean Society of Environmental Toxicology & Chemistry	2024
President's Award, graduation with honors (cum laude), University of Seoul	2024