

SEOJIN KIM

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RESEARCH INTEREST

My research goal is to build the foundational AI system for drug discovery. To this end, I worked on AI-based molecular representation learning and molecular generation. I also worked on the AI security system, such as ensuring certified robustness against adversarial attacks.

- **AI for drug discovery**

TMLR'24, ICML'24, NeurIPS'24

- **Robust AI system**

AAAI'23, TMLR'24

EDUCATION

Seoul National University, J.D. in School of Law

Mar. 2025 - Present

KAIST, M.S. in Artificial Intelligence (completed Ph.D. coursework without completing a dissertation) - Advisor: Prof. Jinwoo Shin

Sep. 2021 - Feb. 2025

KAIST, B.S. in Chemistry (major) & Mathematics (double major) & Computer Science (double major) - Ranked 1st Overall in the Chemistry Department, Summa Cum Laude (GPA: 4.08/4.3)

Mar. 2016 - Aug. 2021

PUBLICATIONS

C: conference, J: journal, W: workshop / * equal contribution

[C2] Data-Efficient Molecular Generation with Hierarchical Textual Inversion

Seojin Kim, Jaehyun Nam, Sihyun Yu, Jinwoo Shin

International Conference on Machine Learning (ICML), 2024

[C1] Confidence-aware Training of Smoothed Classifiers for Certified Robustness

Jongheon Jeong*, Seojin Kim*, Jinwoo Shin

AAAI Conference on Artificial Intelligence (AAAI), 2023 - oral presentation

[J2] Confidence-aware Denoised Fine-tuning of Off-the-shelf Models for Certified Robustness

Suhyeok Jang*, Seojin Kim*, Jinwoo Shin, Jongheon Jeong

Transactions on Machine Learning Research (TMLR), 2024

[J1] Holistic Molecular Representation Learning via Multi-view Fragmentation

Seojin Kim*, Jaehyun Nam*, Junsu Kim, Hankook Lee, Sungsoo Ahn, Jinwoo Shin

Transactions on Machine Learning Research (TMLR), 2024

[W1] An Efficient Tokenization for Molecular Language Models

Seojin Kim, Jaehyun Nam, Jinwoo Shin

NeurIPS Workshop for New Drug Modalities (NeurIPS AIDrugX), 2024

HONORS & AWARDS

Dean's List in the School of Freshman, Fall 2016

Dean's List in the Department of Chemistry, Spring 2017 and Fall 2017

KAIST Presidential Fellowship (KPF), 2018

Dean's List in the College of Natural Science, 2019

ICML Google Travel Grant (\$1,500), 2024

EXPERIENCES

Internship: Institute for Basic Science (IBS), 2017

Internship: SK Hynix HARC Etch Team, 2019

Visiting student: Technische Universität München (Technical University of Munich), 2019

Research project: "Neural Differential Equation for Stock Data Prediction" (advisor: Prof. Jinwoo Shin), 2021