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, NeurIPSW'24
- **Robust AI system**
  AAAI'23, TMLR'24

EDUCATION

KAIST, M.S./Ph.D. in Artificial Intelligence (advisor: Prof. Jinwoo Shin) Sep. 2021 - Present
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 Represnetaion 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

SERVICES

Internship: Institute for Basic Science (IBS), 2017
Internship: SK Hynix HARC Etch Team, 2019
Research project: "Neural Differential Equation for Stock Data Prediction" (advisor: Prof. Jinwoo Shin), 2021
Invited talk: "AI-based Molecular Representation Learning & Generation" in POSTECH, 2023
Domestic patent: "Training Method and Apparatus for Adversarial Robustness of Neural Network Model", 2024
Conference reviewer: ICML (2023, 2024), NeurIPS (2023, 2024), ICLR (2024, 2025), AISTATS (2023)
Journal reviewer: TMLR (2024)