

Seul Lee

CONTACT INFORMATION

KAIST, Seoul, South Korea
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RESEARCH INTERESTS

My research interest is mainly in developing generative models for graphs. I especially focus on molecule generation that can bridge the gap between real-world drug discovery and automatic drug discovery. I am currently interested in the following topics:

- Drug discovery
- Generative models, especially score-based diffusion models
- Graph representation learning

EDUCATION

KAIST, Seoul, South Korea

Ph.D. student, Graduate School of AI **Sep. 2022 - present**

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning
- Expected graduation date: Aug. 2026

M.S., Graduate School of AI **Mar. 2021 - Aug. 2022**

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning

B.S., Department of Aerospace Engineering **Mar. 2015 - Aug. 2019**

B.S., Department of Biological Sciences **Mar. 2015 - Aug. 2019**

RESEARCH EXPERIENCE

AITRICS, Seoul, South Korea

- Position: Research intern
- Research topic: Docking-optimized molecule generation using reinforcement learning

CONFERENCE PUBLICATIONS

[c3] **Score-based Generative Modeling of Graphs via the System of Stochastic Differential Equations**

Jaehyeong Jo*, **Seul Lee***, and Sung Ju Hwang (*: equal contribution),
International Conference on Machine Learning (ICML), **2022**.

	<p>[c2] Edge Representation Learning with Hypergraphs Jaehyeong Jo*, Jinheon Baek*, Seul Lee*, Dongki Kim, Minki Kang, and Sung Ju Hwang (*: equal contribution), Conference on Neural Information Processing Systems (NeurIPS), 2021.</p> <p>[c1] Hit and Lead Discovery with Explorative RL and Fragment-based Molecule Generation Soojung Yang, Doyeong Hwang, Seul Lee, Seongok Ryu, and Sung Ju Hwang, Conference on Neural Information Processing Systems (NeurIPS), 2021.</p>
JOURNAL PUBLICATIONS	<p>[j1] Robotic Scanning Technology for Laser Pulse-Echo Inspection Seul Lee, Jong-min Hyun, Hasan Ahmed, and Jung-ryul Lee, Electronics Letters, 2020.</p>
WORKSHOP PUBLICATIONS	<p>[w1] Exploring Chemical Space with Score-based Out-of-distribution Generation Seul Lee, Jaehyeong Jo, and Sung Ju Hwang, International Conference on Learning Representations Machine Learning for Drug Discovery (ICLR MLDD) Workshop (Oral), 2023.</p>
PREPRINTS	<p>[p1] READRetro: Natural Product Biosynthesis Planning with Retrieval-Augmented Dual-View Retrosynthesis Seul Lee*, Taein Kim*, Min-Soo Choi, Yejin Kwak, Jeongbin Park, Sung Ju Hwang, and Sang-Gyu Kim (*: equal contribution), Nature Communications (Submitted), 2023.</p>
REVIEWER SERVICES	<ul style="list-style-type: none"> • 2022, 2023 International Conference on Machine Learning (ICML) • 2021 Conference on Neural Information Processing Systems (NeurIPS) • 2023 NeurIPS ML4Materials Workshop
HONORS AND AWARDS	<ul style="list-style-type: none"> • Boeing Undergraduate Scholarship Feb. 2018 - Aug. 2019 • KAIST Presidential Fellowship (KPF) Mar. 2017 - Aug. 2019 • National Science and Engineering Scholarship Mar. 2015 - Feb. 2019
REFERENCES	<ul style="list-style-type: none"> • Prof. Sung Ju Hwang, Professor, KAIST <i>E-mail: sjhwang82@kaist.ac.kr</i>