

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**.

[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**.

[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**.

JOURNAL
PUBLICATIONS

[J1] **Robotic Scanning Technology for Laser Pulse-Echo Inspection**
Seul Lee, Jong-min Hyun, Hasan Ahmed, and Jung-ryul Lee,
Electronics Letters, **2020**.

WORKSHOP
PUBLICATIONS

[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**.

PREPRINTS

[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),
Under review, 2023.

REVIEWER
SERVICES

- 2022, 2023 International Conference on Machine Learning (ICML)
- 2021 Conference on Neural Information Processing Systems (NeurIPS)
- 2023 NeurIPS ML4Materials Workshop

HONORS AND
AWARDS

- 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

- **Prof. Sung Ju Hwang**, Professor, KAIST
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