

## Seul Lee

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### CONTACT INFORMATION

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### RESEARCH INTERESTS

My research interest is mainly in developing an automated discovery framework for organic molecules, natural products, or proteins. 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:

- AI for science
- Drug discovery
- Generative 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
- GPA: 4.20/4.3

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

- Double Major in Biological Sciences
- GPA: 4.18/4.3

### RESEARCH EXPERIENCE

**NVIDIA Research** **Feb. 2024 - Aug. 2024**

- Location: Santa Clara, CA, US (remote)
- Position: Research intern
- Research topic: Fundamental generative AI

**Kimlab & The Matter Lab**, UofT **Jun. 2023 - Jun. 2023**

- Location: Toronto, Canada
- Position: Visiting researcher
- Host: Prof. Philip M. Kim & Prof. Alán Aspuru-Guzik

	<b>AITRICS</b>	<b>Jan. 2021 - Feb. 2021</b>
	<ul style="list-style-type: none"> <li>• Location: Seoul, South Korea</li> <li>• Position: Research intern</li> <li>• Research topic: Docking-optimized molecule generation using RL</li> </ul>	
	<b>Opto-Electro-Robotics Lab, KAIST</b>	<b>Mar. 2019 - Aug. 2019</b>
	<ul style="list-style-type: none"> <li>• Location: Daejeon, South Korea</li> <li>• Position: Undergraduate researcher</li> <li>• Advisor: Prof. Jung-ryul Lee</li> <li>• Research topic: Laser pulse-echo inspection with robot arms</li> </ul>	
INVITED TALKS	<ul style="list-style-type: none"> <li>• Exploring Chemical Space with Score-based OOD Generation, Hyundai 2023 R&amp;D AI Conference</li> <li>• Exploring Chemical Space with Score-based OOD Generation, University of Toronto</li> <li>• Score-based Generative Modeling of Graphs via the SDEs, LoGaG: Learning on Graphs and Geometry Reading Group</li> <li>• Learning with Graph-structured Data, POSTECH</li> <li>• Score-based Graph Generation for Material Design, Samsung Advanced Institute of Technology (SAIT)</li> </ul>	<b>Nov. 2023</b> <b>Jun. 2023</b> <b>Oct. 2022</b> <b>Jul. 2022</b> <b>Jun. 2022</b>
CONFERENCE PUBLICATIONS	<p>[c4] <b>Exploring Chemical Space with Score-based Out-of-distribution Generation</b>  Seul Lee, Jaehyeong Jo, and Sung Ju Hwang,  International Conference on Machine Learning (ICML), 2023.</p> <p>[c3] <b>Score-based Generative Modeling of Graphs via the System of Stochastic Differential Equations</b>  Jaehyeong Jo*, Seul Lee*, and Sung Ju Hwang (*: equal contribution),  International Conference on Machine Learning (ICML), 2022.</p> <p>[c2] <b>Edge Representation Learning with Hypergraphs</b>  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] <b>Hit and Lead Discovery with Explorative RL and Fragment-based Molecule Generation</b>  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] <b>Robotic Scanning Technology for Laser Pulse-Echo Inspection</b>  Seul Lee, Jong-min Hyun, Hasan Ahmed, and Jung-ryul Lee,  Electronics Letters, 2020.</p>	

WORKSHOP  
PUBLICATIONS

- [w2] **A Simple and Scalable Representation for Graph Generation**  
Yunhui Jang, **Seul Lee**, and Sungsoo Ahn,  
Conference on Neural Information Processing Systems New Frontiers in Graph  
Learning (**NeurIPS GLFrontiers**) **Workshop, 2023.**
- [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

- [p3] **Drug Discovery with Dynamic Goal-aware Fragments**  
**Seul Lee**, Seanie Lee, and Sung Ju Hwang,  
**Under Review, 2023.**
- [p2] **A Simple and Scalable Representation for Graph Generation**  
Yunhui Jang, **Seul Lee**, and Sungsoo Ahn,  
**Under Review, 2023.**
- [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

- 2024 International Conference on Learning Representations (ICLR)
- 2022, 2023 International Conference on Machine Learning (ICML)
- 2021, 2023 Conference on Neural Information Processing Systems (NeurIPS)
- 2023 Learning on Graphs Conference (LoG)
- 2023 NeurIPS AI4Science Workshop
- 2023 NeurIPS Generative AI & Biology Workshop
- 2023 ICLR 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**, KAIST  
*E-mail: sjhwang82@kaist.ac.kr*