Seonghwan Seo

Ph.D. Candidate | Korea Advanced Institute of Science and Technology
shwan0106@kaist.ac.kr | Website | Google Scholar | GitHub

RESEARCH INTERESTS

Deep Learning
Generative Flow Network (GFlowNet); Graph Neural Network; 3D voxel image modeling

Drug Discovery
Small molecule drug design; Synthesizability; Protein-ligand interaction; Virtual screening; Pharmacophore modeling

EDUCATION

Korea Advanced Institute of Science and Technology (KAIST) Daejeon, South Korea
Ph.D. student in Chemistry *Aug. 2022 - Feb. 2028 (expected)*
Supervisor: Woo Youn Kim

Korea Advanced Institute of Science and Technology (KAIST) Daejeon, South Korea
B.S. in Chemistry & Computer Science (Double Major) *Feb. 2018 - Aug. 2022*
Supervisor: Young Min Rhee
GPA: 3.99/4.3

EXPERIENCES

Intelligent Chemistry Lab, KAIST Daejeon, South Korea
AI for Drug Discovery *June 2019 - Present*
Supervisor: Woo Youn Kim

- Development of an unbiased drug-likeness scoring
- Development of a DL framework for fully-automated receptor-based pharmacophore modeling
- Development of generative models for drug design
- Research projects on synthesizable drug discovery

HITS Inc. Seoul, South Korea
AI Research Intern *Dec. 2020 - Aug. 2022*
Manager: Jaechang Lim

- Development of reaction template-based generative model for synthesizable molecular design with desired property
- Development of transformer-based model for synthesis path generation

PUBLICATIONS

* indicates equal contribution

- Compositional Flows for 3D Molecule and Synthesis Pathway Co-design
  Tony Shen*, **Seonghwan Seo***, Ross Irwin, Kieran Didi, Simon Olsson, Woo Youn Kim, Martin Ester
  ICLR 2025 AI4Mat Workshop (Spotlight); GEM Workshop (Spotlight), 2025 (TBA)
- Generative Flows on Synthetic Pathway for Drug Design [link]
  Seonghwan Seo, Minsu Kim, Tony Shen, Martin Ester, Jinkyoo Park, Sungsoo Ahn, Woo Youn Kim
  International Conference on Learning Representations (ICLR), 2025
- PharmacoNet: deep learning-guided pharmacophore modeling for ultra-large-scale virtual screening [link]
  Seonghwan Seo, Woo Youn Kim
  Chemical Science, 2024
- TacoGFN: Target Conditioned GFlowNet for Structure-based Drug Discovery [link]
  Tony Shen, **Seonghwan Seo**, Grayson Lee, Mohit Pandey, Jason R Smith, Artem Cherkasov, Woo Youn Kim, Martin Ester
  Transactions on Machine Learning Research (TMLR), 2024
- Molecular Generative Model via Retrosynthetically Prepared Chemical Building Block Assembly [link] [cover]

Seonghwan Seo, Jaechang Lim, Woo Youn Kim
Advanced Science, 2023 (selected for a journal cover)

- Drug-likeness scoring based on unsupervised learning [link]
  Kyunghoon Lee*, Jinho Jang*, **Seonghwan Seo***, Jaechang Lim, Woo Youn Kim
  Chemical Science, 2022

PRESENTATIONS

Invited

- "Molecular Generative Model via Retrosynthetically Prepared Chemical Building Block Assembly"
  Oral workwhop and tutorial at *AI-BIO, Artificial Intelligence Institute, Seoul National University*, Seoul, South Korea (Nov. 2022)

Contributed

- "Generative Flows on Synthetic Pathway for Drug Design"
  Poster presentation at *NeurIPS Workshop on AI for New Drug Modalities 2024*, Vancouver, Canada. (Dec. 2024)
- "PharmacoNet: Accelerating Large-Scale Virtual Screening by Deep Pharmacophore Modeling"
  Poster presentation at *NeurIPS 2023 Workshop on New Frontiers of AI for Drug Discovery and Development (AI4D3)*, New Orleans, LA, USA. (Dec. 2023)
- "Molecular Generative Model via Retrosynthetically Prepared Chemical Building Block Assembly"
  Poster presentation at *2023 Accelerate Conference*, Toronto, Canada (Aug. 2023)

AWARDS & SCHOLARSHIPS

- **Awards: Admission in Graduate School with Highest Honors**
  KAIST Chemistry Alumni Association, 2023
- **KAIST Alumni Scholarship**
  KAIST Alumni Association, 2021 - 2022
- **Younghoon Lee Scholarship**
  Department of Chemistry, KAIST, 2021
- **Model Student Awards**
  KAIST, 2021
- **Dean's List**
  College of Natural Science, KAIST, 2021
- **National Science & Technology Scholarship**
  Government of South Korea, 2020 - 2021
- **Dean's List**
  School in Freshman, KAIST, 2019

ACADEMIC REVIEWER

- International Conference on Learning Representation (ICLR), 2025
- Nature Communication, 2024

SKILLS

Languages

Korean (native), English (upper-intermediate)

Deep Learning Tools

Python, PyTorch, PyTorch Geometric, PyTorch Lightning, Numba, Pandas

Chemistry Tools

RDKit, OpenBabel, Vina, Smina, rDock