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); 3D voxel image modeling

Drug Discovery
Protein; Small molecule; Drug Design; Protein-ligand interaction; Pharmacophore modeling; Virtual screening; Molecular design;
Property prediction; Molecular docking

Material Discovery
Property-control; Synthesizability

EDUCATION

Korea Advanced Institute of Science and Technology (KAIST) Daejeon, South Korea
Ph.D. student in Chemistry *Aug. 2022 - Aug. 2027 (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 Research Assistant, AI-based drug discovery *June 2019 - Present*
Supervisor: Woo Youn Kim

- Designing the deep learning framework for a new drug-likeness scoring
- Development of deep learning model for fully-automated receptor-based pharmacophore modeling
- Research projects on high-throughput structure-based virtual screening
- Research projects on pharmacophore-guided generative model for target-aware molecular design

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 SMILES generative model by synthesis path generation
- Research Projects on protein-ligand binding pose prediction with score-based model

PUBLICATIONS

* indicates equal contribution

Journals

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

Conferences

- PharmacoNet: Accelerating Large-Scale Virtual Screening by Deep Pharmacophore Modeling [link]
  Seonghwan Seo, Woo Youn Kim
  NeurIPS 2023 Workshop on New Frontiers of AI for Drug Discovery and Development (AI4D3), 2023

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

- "PharmacoNet: Accelerating Large-Scale Virtual Screening by Deep Pharmacophore Modeling" Poster presentation at the *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 the *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

PROFESSIONAL SERVICES

Open-sourced Software Development

- MolVoxel: Easy-to-use molecular voxelization tool with minimal dependencies [link]
- OpenPharmaco: Open-source GUI tools for protein-based pharmacophore modeling and virtual screening [link]

SKILLS

Languages

Korean (native), English (upper-intermediate)

Deep Learning Tools

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

Chemistry Tools

RDKit, OpenBabel, Smina, rDock