

# Seonghwan Seo

Ph.D. Candidate | Korea Advanced Institute of Science and Technology

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## RESEARCH INTERESTS

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### Deep Learning

Generative model; GFlowNet; XAI; Multi-modal; Graph neural network; 3D voxel image modeling

### Drug Discovery

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

### Material Discovery

Property-control; Synthesizability

## EDUCATION

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### Korea Advanced Institute of Science and Technology (KAIST)

Ph.D. student in Chemistry

Supervisor: Woo Youn Kim

Daejeon, South Korea

Aug. 2022 - Aug. 2027 (expected)

### Korea Advanced Institute of Science and Technology (KAIST)

B.S. in Chemistry & Computer Science (Double Major)

Supervisor: Young Min Rhee

GPA: 3.99/4.3

Daejeon, South Korea

Feb. 2018 - Aug. 2022

## EXPERIENCES

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### Intelligent Chemistry Lab, KAIST

AI Research Assistant, AI-based drug discovery

Supervisor: Woo Youn Kim

Daejeon, South Korea

June 2019 - Present

- 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.

AI Research Intern

Manager: Jaechang Lim

Seoul, South Korea

Dec. 2020 - Aug. 2022

- 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

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\* indicates equal contribution

### Journals

- 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

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### Invited

- "Molecular Generative Model via Retrosynthetically Prepared Chemical Building Block Assembly" Oral workshop 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. (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

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- **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

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### Open-sourced Software Development

- MolVoxel: Easy-To-Use Molecular Voxelization Tool with Minimal Dependencies [[link](#)]

## SKILLS

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### Languages

Korean (native), English (upper-intermediate)

### Deep Learning Tools

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

### Chemistry Tools

RDKit, OpenBabel, Smina, rDock