Seokhyun Moon

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Research Interests

Molecular Interaction Modeling for Drug Discovery and Applications
My research began with protein–ligand interaction prediction. In PIGNet and PIGNet2, I developed physics-informed models for binding affinity scoring and virtual screening, with a focus on generalization to unseen systems. I then moved from scoring given structures to predicting the structures themselves, working on co-folding and biomolecular complex structure prediction; I am one of the main developers of **K-Fold**, which models complex formation as a transition from the unbound components to the bound state. In parallel, I am interested in molecular generative models for lead optimization and *de novo* drug design. More recently, I have been working on **agentic frameworks** that aim to overcome the limitations of conventional single-target-based *in silico* drug discovery, and I am also interested in phenotypic drug discovery using virtual cells.

Positions

Korea Advanced Institute of Science and Technology (KAIST), InnoCORE — Sep 2026 – Present
Postdoctoral Researcher

Education

Korea Advanced Institute of Science and Technology (KAIST), Ph.D. in Chemistry — Sep 2020 – Aug 2026
Advisor: Woo Youn Kim

Korea Advanced Institute of Science and Technology (KAIST), BS in Chemistry — Mar 2017 – Aug 2020

Publications

(*: Equal Contribution, †: Corresponding Author)

Predicting conformational changes induced by biomolecular interactions — 2026

Yeongnam Bae, Jinheon Baek, Eugene Choi, . . . , Hyeongwoo Kim†, . . . , **Seokhyun Moon**, . . . , Woo Youn Kim†, Gyu Rie Lee, and Byung-Ha Oh

K-Fold. One of the main developers: co-designed the diffusion bridge module and led its development.

[P2] bioRxiv preprint | Code

AtlasFold: Protein structure prediction with metagenomic-scale language models — 2026

Seonghwan Seo†, Hyeongwoo Kim, **Seokhyun Moon**, Woo Youn Kim†, and Team KAIST

[P1] bioRxiv preprint | Code

Autonomous bioisosteric replacement for multi-property optimization in drug design — 2026

Hyeongwoo Kim*, **Seokhyun Moon***, Wonho Zhung, Shinwoo Kim, Jaechang Lim, and Woo Youn Kim†

[J5] Nature Communications 17, 9113 | Code

How Do Co-folding Models Organize Structural Information? — 2026

Minha Park*, Shinwoo Kim*, **Seokhyun Moon**, Hyeongwoo Kim, Gyuho Jeon, and Woo Youn Kim†

[W4] ICML 2026 Workshop: GenBio | bioRxiv preprint

FragFM: Hierarchical Framework for Efficient Molecule Generation via Fragment-Level Discrete Flow Matching — 2026

Joongwon Lee*, Seonghwan Kim*, **Seokhyun Moon***, Hyunwoo Kim†, and Woo Youn Kim†

[C3] ICLR 2026 | Code

MoAgent: A Hypothesis-Driven Multi-Agent Framework for Drug Mechanism of Action Discovery — 2025

Jun Hyeong Kim, **Seokhyun Moon**, Seonghwan Kim, Junhyeok Jeon, Taein Kim, Jisu Seo, Songmi Kim, and Woo Youn Kim†

[W2] NeurIPS 2025 Workshop: AI4D3, [W3] NeurIPS 2025 Workshop: FM4LS | Code

Discrete Diffusion Schrödinger Bridge Matching for Graph Transformation 2025
Jun Hyeong Kim*, Seonghwan Kim*, **Seokhyun Moon***, Hyeongwoo Kim*, Jeheon Woo*, and Woo Youn Kim†
[C2] ICLR 2025, [W1] NeurIPS 2024 Workshop: AI for New Drug Modalities | Code

Toward Generalizable Structure-Based Deep Learning Models for Protein-Ligand Interaction Prediction: Challenges and Strategies 2024
Seokhyun Moon*, Wonho Zhung*, and Woo Youn Kim†
[J4] WIREs Computational Molecular Science

PIGNet2: A Versatile Deep Learning-based Protein-Ligand Interaction Prediction Model for Binding Affinity Scoring and Virtual Screening 2024
Seokhyun Moon, Sang-Yeon Hwang, Jaechang Lim, and Woo Youn Kim†
[J3] Digital Discovery | Code

GeoTMI: Predicting Quantum Chemical Property with Easy-to-Obtain Geometry via Positional Denoising 2023
Hyeonsu Kim*, Jeheon Woo*, Seonghwan Kim*, **Seokhyun Moon***, Jun Hyeong Kim*, and Woo Youn Kim†
[C1] NeurIPS 2023 | Code

PIGNet: a physics-informed deep learning model toward generalized drug-target interaction prediction 2022
Seokhyun Moon*, Wonho Zhung*, Soojung Yang*, Jaechang Lim, and Woo Youn Kim†
[J2] Chemical Science | Code

Scaffold-based molecular design with a graph generative model 2020
Jaechang Lim*, Sang-Yeon Hwang*, **Seokhyun Moon**, Seungsu Kim, and Woo Youn Kim†
[J1] Chemical Science | Code

Invited Talks

Developing a generative model of protein-ligand complexations
AI Star Fellowship Workshop (KAIST Graduate School of AI, Seoul, South Korea) Nov 2025
Symposium on AI New Drug Development Using Ultra-High Performance Supercomputing (MOGAM Institute for Biomedical Research, Seoul, South Korea) Oct 2025

Awards

President's Award, Telecommunications Technology Association (AI-Champion) 2025
Recipient, 10th EDISON Computational Chemistry software application competition 2020

Recipient, KAIST Undergraduate Research Program participation prize 2020
Recipient, Qualcomm-KAIST Innovation Awards 2019

Academic Services

Conference reviewer

- International Conference on Learning Representations (**ICLR**), 2025, 2026
- International Conference on Learning Representations (**ICLR**), GEM workshop, 2024
- Neural Information Processing Systems (**NeurIPS**), 2025

Teaching Experience

Teaching Assistant

- CH102: General Chemistry Major Lab I (Computational Chemistry), KAIST, 2024 (Spring, Fall)
- CH252: Chemistry Major Lab I (Computational Chemistry), KAIST, 2020 (Fall), 2022 (Fall)