Jiho Sim

PhD Candidate, Seoul National University

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Research Interests

Primary Interaction between biomolecules (affinity and structure prediction), Biomolecular Foundation Models, Ligand/Protein design

Keywords Structural biology, Computational chemistry, Deep learning, Biomolecular engineering, Drug discovery

Future Directions Integration of biomolecular and genomics foundation models into a virtual cell; understanding biology based on interactions; defining the *Foundation Model* of biology

Education

2021–Present **Ph.D. in Chemistry (Direct PhD Program; B.S. completed 2021)**, *Seoul National University*, Seoul, South Korea
- Advisor: Prof. Chaok Seok (Lab of Computational Biology and Biomolecular Engineering)
- Research Focus: Protein-ligand interactions and foundation models for biomolecules
- Expected Graduation: 2026

2016–2021 **B.S. in Chemistry**, *Seoul National University*, Seoul, South Korea
- Graduated *cum laude*
- Outstanding Bachelor's Thesis Award

Publications

Peer-Reviewed Journal Articles

2023 **Jiho Sim**, Sohee Kwon, Chaok Seok. (2023). "HProteome-BSite: predicted binding sites and ligands in human 3D proteome." *Nucleic Acids Research*.

2023 Won Hoon Choi, Yejin Yun, Insuk Byun, Sumin Kim, Seho Lee, **Jiho Sim**, Shahar Levi, Seo Hyeong Park, Jeongmoo Jun, Oded Kleifeld, Kwang Pyo Kim, Dohyun Han, Tomoki Chiba, Chaok Seok, Yong Tae Kwon, Michael H. Glickman, Min Jae Lee. (2023). "ECPAS/Ecm29-mediated 26S proteasome disassembly is an adaptive response to glucose starvation." *Cell Reports*.

2025 Seeun Kim, Simaek Oh, Hyeonuk Woo, **Jiho Sim**, Chaok Seok, Hahnbeom Park. (2025). "Deep learning molecular interaction motifs from receptor structure alone." *Journal of Cheminformatics*.

Preprints & Manuscripts Under Review

2025 **Jiho Sim**, Chaok Seok, Hahnbeom Park. (2025). "MotifScreen: Generalizing Virtual Screening through Learning Protein-Ligand Interaction Principles." *preprint*.

Research Experience

2021–Present **Graduate Research Assistant**, *Laboratory of Prof. Chaok Seok*, Seoul National University, Seoul, South Korea

- Developed deep learning methods, including **MotifScreen**, for predicting molecular interaction motifs from receptor structures and applying them to precise interaction prediction (under submission).
  - This project reinforced the importance of high-quality training and test data, and demonstrated how careful problem formulation directly impacts model performance—principles I actively applied throughout the work.
- Built protein-ligand affinity prediction models using large-scale structural and interaction datasets, including the role of *water molecules*.
- Coordinated the development of the foundation model **GalaxyMol** for biomolecular complex modeling.
  - Curated comprehensive benchmarks to evaluate GalaxyMol's ability to capture protein conformational changes.
  - GalaxyMol is a generative diffusion-based model, extended from the Boltz architecture with novel contributions.
- Built **HProteome-BSite**, a database and prediction tool for binding sites and ligands in the human 3D proteome (*Nucleic Acids Research*, 2023).
- Contributed to interdisciplinary projects integrating structural biology, computational chemistry, and AI/ML.

2020.09–2021.02 **Undergraduate Research Assistant**, *Computational Chemistry Laboratory*, Seoul National University, Seoul, South Korea

- Advisor: Prof. Chaok Seok
- Bachelor's Thesis: "Structure Prediction and Ligand Docking of Oxytocin Receptor and Vasopressin Receptor Using Computational Methods"
- Outstanding Bachelor's Thesis Award

2019.02–2019.08 **Undergraduate Research Assistant**, *Structural Biochemistry Laboratory*, Seoul National University, Seoul, South Korea

- Advisor: Prof. Hyung Ho Lee
- Project: "Expression and Purification of FOXL2/XRCC6 Complex Regulating DSB Repair in NHEJ System"

Presentations

Invited Symposium Talks

2025 "Developing AI Tools for Protein-Ligand Interaction Prediction: Discovering Novel Compounds for Target Proteins and Scaling Predictions to Proteomics." APEC Young Chemistry Leaders' Forum -Embracing a New Era of Digital Transformation in Chemistry 3, Korean Chemical Society 135th Conference (April 23-25, 2025).

Poster Presentations

2025.07 MotifScreen: Revolutionizing virtual screening and its generalizability via deep learning of interaction patterns. 2025 Summer KIDDS Conference. **Outstanding Poster Award**

2025.03 Docking-free Structure-based Virtual Screening Neural Network using Multimodal Training. SNU Department of Chemistry Graduate Student Poster Presentation and Research Exchange Meeting. **Outstanding Poster Award**

2024.12 Enhancing Structure and Affinity Prediction of Receptor-Ligand Interactions with Variable Receptor Flexibilities Using Deep Learning Methods. CASP16.

2023.08 Developing a ligand- and structure-based virtual screening method using SE(3) transformer and trigonometry attention. ACS Fall 2023.

2022.09 Predicting ligand interactions for human 3D proteome. Joint Meeting of the 20th KIAS Conference on Protein Structure and Function and The 7th Korean-Polish Conference.

Scholarships & Fellowships

2023–2025 Asan Scholarship for Graduate Students in Biomedical Sciences (국내의생명과학분야대학원장학생), Asan Foundation

2019 Joo Jung-Kwang Heo Ji-Young Scholarship (주중광허지영장학금), Undergraduate academic excellence award

Technical Skills

AI/ML & Programming: Python, Bash scripting, PyTorch, PyTorch Lightning, PyTorch Geometric, multi-GPU distributed training, Transformers, SE(3) networks, multimodal AI

Bio/Chem Informatics: RDKit, ChimeraX, Biotite, biomolecular file formats (PDB, CIF, MOL2, SDF, etc.)

Tools & Systems: Git (collaborative development), HPC clusters with Slurm workload management

Software & Databases

2025 **MotifScreenK (MSK)**, *Virtual Screening Tool*, API server

- Initial version of MotifScreen (deep learning-based virtual screening method)
- Optimized for kinase families such as ROCK1
- Website: `https://galaxy.seoklab.org/kaidd` (see "submit msk")
- Part of KAIDD package (K-Artificial Intelligence Drug Discovery, `www.kaidd.re.kr`)

2022 **HProteome-BSite**, *Database and Prediction Tool*

- Comprehensive database of predicted binding sites and ligands for human proteins
- Freely accessible for researchers in drug discovery and structural biology
- Website: `https://galaxy.seoklab.org/hproteome-bsite/database/`
- Published in *Nucleic Acids Research*, 2023

Languages

Korean Native

English Fluent — *Academic and professional proficiency*

Japanese Conversational — *Able to discuss research topics*

References

Primary Advisor

Dr. Chaok Seok
Professor
Department of Chemistry
Seoul National University
Email: chaok@snu.ac.kr

Co-Advisor

Dr. Hahnbeom Park
Senior Researcher (PI, Lab of Computational Drug Discovery)
Brain Science Institute, KIST
Email: hahnbeom@kist.re.kr

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