

# Jiho Sim

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## Introduction

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PhD candidate, Lab of Computational Biology and Biomolecular Engineering, Seoul National University.

Interested in: **Protein ligand interaction** and **making tools that understand such interactions**.

## Education

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Seoul National University, BS in Chemistry

Mar 2016 – Feb 2021

## Current Projects

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### End-to-end Virtual Screening Model

Mar 2022 –

- Built a virtual screening tool that captures structure information without a heavy docking process.
- Multi-modal training to help model learn important protein ligand interactions.
- Building a more generalizable model with careful data curation of training and test set.
- Initial version of the model is available through web server.

### Foundation Model

Mar 2024 –

- Developing a foundation model for protein structure prediction.
- Foundation model development is a large project within the lab, with teams divided for specific tasks.
- Working as one of the main project coordinators. Led input (protein) featurization and dataset curation.

### Affinity Prediction Model

Jan 2025 –

- Developing a model for affinity prediction that understands more than just protein ligand pairwise interaction.

## Publications

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### HProteome-BSite: predicted binding sites and ligands in human 3D proteome

Jan 2023

*Jiho Sim*, Sohee Kwon, Chaok Seok

10.1093/nar/gkac873

### Deep learning molecular interaction motifs from Receptor structure alone

Jan 2025

Seeun Kim, Simaek Oh, Hyeonuk Woo, *Jiho Sim*, Chaok Seok, Hahnbeom Park  
biorxiv

### ECPAS/Ecm29-mediated 26S proteasome disassembly is an adaptive response to glucose starvation

Jul 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

10.1016/j.celrep.2023.112701

## Honors and Awards

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Asan Scholarship (국내 의생명과학분야 대학원 장학생), Asan Foundation

Mar 2023 - Feb 2025

Best Senior Paper Award (2020년 학부 졸업생 우수논문)

2020

주중광희지영 장학금

2019