

# DAVID HYUNYOO JANG

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## EDUCATION

### Seoul National University

PharmD

- Selected Coursework Biochemistry · Pharmaceutical Statistics · Drug Delivery Systems

Mar 2022 – Feb 2028

Seoul, South Korea

### Korea University

B.Eng. in Materials Science and Engineering

- Selected Coursework Organic Nanomaterials · Fundamentals of Data Science

Mar 2019 – Aug 2021

Seoul, South Korea

## RESEARCH EXPERIENCE

### AI Protein Design Lab, Korea Advanced Institute of Science and Technology (KAIST)

Undergraduate Researcher (advisor: Gyu Rie Lee)

Jun 2025 – Aug 2025

Daejeon, South Korea

- Designed de novo protein binders targeting *phenytoin* and *carbamazepine* using diffusion-based generation and multi-criteria triage (Rosetta interface scores, RMSD/pLDDT metrics from AlphaFold3, Boltz-2, TMalign, PLACER);
- Devised a backbone diversification and optimization strategy via iterative LigandMPNN–FastRelax cycles, which expanded the *carbamazepine* candidate pool (21→275) and improved interface  $\Delta\Delta G$  (–25.4→–31.6 kcal/mol).
- Established a fully reproducible end-to-end binder design pipeline, and released as an open-source repository on GitHub.
- Implemented atom-wise bias conditioning functionality for relative accessible surface area (rASA) in RFdiffusion All-Atom.

### Laboratory of Computational Drug Discovery, Seoul National University

Undergraduate Researcher (advisor: Juyong Lee)

Jul 2023 – Aug 2025

Seoul, South Korea

- Led development of PREpiBind, a transformer-based pMHC-II predictor; ran embedding ablations across AF3/Chai-1/Boltz-1, ESM series, and BLOSUM, selected ESM C Small for the best accuracy–size trade-off, achieved ROAUC 0.998 on MS datasets, and released a public web server (manuscript in prep).
- Benchmarked 27 LLMs on Korean Pharmacist Licensing Exam (2019–2024); built the evaluation framework and error taxonomy; 7 models passed all years, best reaching top-12% of human examinees (manuscript submitted).
- Reproduced a small-molecule discovery pipeline for CB1 receptor using AutoDock-GPU and the Enamine Hit Locator Library, automating QC and ranking scripts for high-throughput screening.

### Structure & Knowledge Injection into Machine Learning Lab, Seoul National University

Undergraduate Researcher (advisor: Jay-Yoon Lee)

May 2024 – Sep 2024

Seoul, South Korea

- Implemented a joint-loss for semi-supervised training in RoseTTAFold2NA, enabling use of unlabeled sequences alongside labeled data; integrated the loss into the training loop (dataloaders/optimizer flow), refactored code for unlabeled batches; validated functionality with ablations across three label-density regimes, confirming stable learning signals.

### Systems Pharmacology Lab, Seoul National University

Undergraduate Intern (advisor: Minsoo Noh)

Jun 2023 – Jul 2023

Seoul, South Korea

- Performed a HaCaT cell-based PGE<sub>2</sub> competitive ELISA to assess tryptophol's anti-inflammatory effects; benchmarked against NSAIDs, analyzed dose–response data.

## TECHNICAL SKILLS

**Programming & Data:** Python, PyTorch, Numpy, Bash, pandas, matplotlib, Streamlit, Nginx, LaTeX

**Modeling & Docking:** RDKit, PyMOL, Chimera, AutoDock, PyRosetta, RFdiffusion (AA), LigandMPNN, AlphaFold3

**Systems & DevOps:** Linux, Git, Slurm, conda/mamba, HuggingFace

**Experimental Techniques:** cell culture (HaCaT), buffer/reagent prep, competitive ELISA, serial dilutions, plate reader

## OTHER EXPERIENCE

### Seoul National University Hospital

Hospital Pharmacy Practicum

Dec 2024 – Feb 2025

Seoul, South Korea

- Dispensing, patient counseling, medication safety workflow.

### E-Blue Pharmacy

Community Pharmacy Practicum

Feb 2025 – Mar 2025

Seoul, South Korea

- Community dispensing, OTC counseling, inventory coordination.

### Military Service

Sergeant

Aug 2025 – Feb 2027

III Corps, Republic of Korea Army

- Operated and maintained portable surface-to-air missile systems during air-defense training and readiness operations.

## LEADERSHIP / EXTRACURRICULAR

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### SNU Alpha (Deep Learning Study Club)

Spring 2022 – Winter 2024

*Executive Member, Co-Founder*

*College of Pharmacy, Seoul National University*

- Peer-taught deep learning basics and applications in drug discovery.
- Led weekly study sessions on Natural Language Processing in Fall 2023 and PyTorch in Spring 2024.
- Managed executive board of 5 members and ran weekly meetings to oversee progress in essential parts of the chapter.

### SNU Boncho (Pharmacy Student–Alumni Association)

Spring 2022 – Winter 2024

*Executive Member*

*College of Pharmacy, Seoul National University*

- Facilitated intergenerational networking among pharmacy students, alumni, and faculty.
- Organized informal gatherings and mentorship sessions bridging undergraduate and professional members.
- Supported planning of alumni events and student outreach activities.

## AWARDS & FUNDING

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### Research Excellence Award, 2024 SNU Student-Directed Education Undergraduate Research Program

2025

*President of Seoul National University*

- Awarded to two projects per fields (ten total) for excellence in research execution and outcomes.

### 2024 SNU Student-Directed Education Undergraduate Research Program

2024

*Faculty of Liberal Education, Seoul National University*

- Selected as one of 36 projects to receive funding for undergraduate research.

## PAPERS AND PRESENTATIONS

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[1] PREpiBind: Protein Representation-integrated Epitope-MHC Class II Binding Prediction

**David Hyunyoo Jang**, Dongwoo Kim, Byungho Park, Untaek Hwang, Yoonjoo Choi, Juyong Lee  
KIDDS 2025 Summer Workshop (Korean In silico bioDesign and Discovery Society, Poster)

*Manuscript in preparation*

[2] Large Language Models Pass the Korean Pharmacist Licensing Examination: A Benchmarking Study

**David Hyunyoo Jang**, Juyong Lee  
Under review

[3] DeepXeno: Structure-Informed Prediction of Xenotransplantation Immunogenicity

**David Hyunyoo Jang**, Byungho Park, Untaek Hwang, Juyong Lee

Outstanding Research Presentation in 2024 SNU Student-Directed Education Undergraduate Research Program (Oral)