# DAVID HYUNYOO JANG

whwjang00@snu.ac.kr in daylight00 ↑ daylight-00 | US Citizen

#### **EDUCATION**

#### **Seoul National University**

Mar 2022 - Feb 2028 (Expected)

PharmD Seoul, South Korea

Selected Coursework: Biochemistry · Pharmaceutical Statistics · Drug Delivery Systems

Korea University Mar 2019 – Aug 2021

Coursework in Materials Science and Engineering (no degree)

Selected Coursework: Organic Nanomaterials · Fundamentals of Data Science

Seoul, South Korea

#### RESEARCH EXPERIENCE

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

Jun 2025 – Aug 2025

Undergraduate Researcher (advisor: Gyu Rie Lee)

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  $(21\rightarrow275)$  and improved interface  $\Delta\Delta G$   $(-25.4\rightarrow-31.6$  *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

Jul 2023 - Aug 2025

Undergraduate Researcher (advisor: Juyong Lee)

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

May 2024 - Sep 2024

Undergraduate Researcher (advisor: Jay-Yoon Lee)

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

Jun 2023 - Jul 2023

*Undergraduate Internship (advisor: Minsoo Noh)* 

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

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**

Dec 2024 - Feb 2025

Hospital Pharmacy Practicum

Seoul, South Korea

• Dispensing, patient counseling, medication safety workflow.

## E-Blue Pharmacy

Feb 2025 - Mar 2025

Community Pharmacy Practicum

Seoul, South Korea

• Community dispensing, OTC counseling, inventory coordination.

#### **Military Service**

Aug 2025 - Feb 2027 (Expected)

Sergeant

III Corps, Republic of Korea Army

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

#### LEADERSHIP / EXTRACURRICULAR

#### **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.

#### 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**

**Research Excellence Award**, 2024 SNU Student-Directed Education Undergraduate Research Program *President of Seoul National University* 

2025

• 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

- [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)