Haelee Bae

CONTACT INFORMATION

AI Graduate School, Gwangju Institute of Science and Technology(GIST), Republic of Korea

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Actively seeking a focused 2-month internship (Dec 2025 - Feb 2026) in AI-driven drug discovery to apply my deep learning based research to real world settings. This experience also fulfills the graduation requirement of my Ph.D program at GIST.

INTERESTS

Deep learning for RNA- and Protein-targeted drug discovery

RNA-Compound and Protein-Compound interaction prediction

Generative model for small molecules

Active learning, Uncertainty Quantification, Foundation models, Multi agent systems

EDUCATION

Ph.D Candidate in AI Graduate School, GIST, Korea (expected Aug 2026)

■ **Research area: Deep learning based RNA targeted small molecule prediction and generation**

M.S in School of Electrical Engineering and Computer Science, 2021, GIST, Korea

■ Thesis: Drug target binding affinity prediction considering the interaction of molecule atom and protein subsequences

B.S in Computer Science and Engineering, 2019, Hanyang University, ERICA, Korea

■ Exchange Student in Arizona State University (2018 Fall)

PUBLICATIONS

Bae, Haelee, and Hojung Nam*. "A Deep Learning Approach for RNA-Compound Interaction Prediction with Binding Site Interpretability." *Under Revision*

Bae, Bongsung, Haelee Bae, and Hojung Nam*. "LOGICS: Learning optimal generative distribution for designing de novo chemical structures." *Journal of Cheminformatics 15.1 (2023): 77.*

Bae, Haelee, and Hojung Nam*. "GraphATT-DTA: attention-based novel representation of interaction to predict drug-target binding affinity." *Biomedicines 11.1 (2022): 67.*

CONFERENCE

Bae, Haelee, Bongsung Bae, and Hojung Nam*. "De novo RNA binding compound generation via reinforcement learning guided by Bayesian uncertainty based reward" *ISMB 2025*

Bae, Haelee, and Hojung Nam*. "Uncertainty-aware deep learning model for RNA-Compound Interaction Prediction" *RECOMB 2025*

Bae, Haelee, and Hojung Nam*. "A Deep Learning Approach for RNA-Compound Interaction Prediction with Binding Site Interpretability" *NeurIPS 2024 Workshop on AI for New Drug Modalities.*

HONOR and AWARDS

Inseong Hongboksoon Scholarship, GIST 2021.11

Dream AI Grand Prize, NVIDIA and GIST 2020.12

Full Government Scholarship, GIST 2019.09 -present

Capstone Design Grand Prize, Hanyang University 2019.06

Super challenge hackathon Great Prize, Inha University 2018.02

PROJECTS

AI-based discovery of novel acromegaly-specific targets and development of innovative therapeutics based on RNA degradation, *Ministry of Science and ICT* 2025-2029

- Student Researcher
- Develop deep learning models for predicting RNA-compound interaction and binding site
- Design generative models for novel RNA binding small molecule

Deep learning based small molecule discovery for allergic disease, *Korea Institute for Advancement of Technology (KIAT)* 2021-2022

- Student Researcher
- Trained protein-compound interaction prediction model
- Performed virtual screening of candidate molecules and analyze protein binding site

Big data & AI-based drug development acceleration platform development, *Korea Institute of Human Resources Development in Science and Technology* 2021

- Student Researcher
- Developed drug protein interaction prediction model
- Conducted gradient based compound space exploration for PK/PD optimization using a pre-trained VAE model

ACTIVITIES

Lectures on AI-driven Drug discovery (LAIDD) mentoring project, *Korean Pharmaceutical and Bio-Pharma Manufacturers Association* 2024.08 - 2024.11

- Teaching Assistant
- Assisted mentoring and lectures on AI-based drug discovery
- Guided mentees on dataset curation, modeling techniques, performance evaluation and poster preparation

Health Data Academy, *Arizona State University, Columbia University and Icahn School of medicine* 2018.12

SKILLS

Programming: Python, Pytorch, DGL, PyG, RDkit, Scikit-learn

Languages: Korean (Native), English (TOEFL IBT 90, TOEIC: 895)