Dongmin (Eugene) Bang (he/him)

Pharm.D, Ph.D Candidate in Bioinformatics *(Expected Aug. 2025)*

Personal Information

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Summary

- **PharmD and PhD candidate in Bioinformatics**, positioned at the intersection of systems pharmacology and machine learning, with interests in knowledge-guided and data-driven modeling of biological systems for AI-augmented therapeutic design.
- Contributed to 16 peer-reviewed publications (9 first/co-first author) during doctoral study, including **first-author papers in *Nature Communications*, ISMB, and ICML,** on integrative modeling of gene regulation, drug perturbation responses, and representation learning across biomedical modalities to simulate systemic therapeutic responses.
- Completed a **competitive, university-funded research grant** (Advanced Medical Researcher Training Program–Seoul National University), leading an independent project on **transfer learning for virtual drug-induced cell state transition and multi-scale drug response prediction**, resulting in a **first-authored ISMB 2024 publication.**
- Mentored interns and junior researchers, contributing to **four co-first-author publications in *Journal of Cheminformatics* and ISMB 2025**, and multiple collaborative works across multi-modal representation learning, molecular modeling, and network biology.
- Led an **AI-driven drug discovery team** in industry, collaborating with hospitals, biotech startups, and medicinal chemistry groups to integrate omics-informed modeling, perturbation response simulation, and medicinal chemistry insights for *in silico* target prioritization and candidate optimization.

Education

03/2021–Present **Ph.D Candidate in Bioinformatics** *(Expected Aug. 2025)*
Seoul National University, Seoul, Republic of Korea.
Advisor: Prof. Sun Kim
Dissertation: *Towards Computational Integration of Multi-scale Biomedical Interactions for Precision Medicine: from Data to Knowledge*
– Dissertation proposal approved with minor committee comments.

03/2015–02/2021 **Pharm.D, College of Pharmacy**
Chung-Ang University, Seoul, Republic of Korea.

03/2012–02/2015 **B.S.E student in Architectural Engineering**
Hanyang University, Seoul, Republic of Korea.

Professional Experiences

Research Experience

09/2022–Current **AIGENDRUG Co., Ltd.**, Seoul, Republic of Korea
Position: Senior Research Scientist, AI-Drug Discovery Team

Role: Led an AIDD team in constructing AI-integrated new-modality drug discovery pipelines, collaborating with academia, hospital, biotech and pharmaceutical companies, and patenting two frameworks (ROK patent, granted).

Selected Publications (Full list available in the Appendix)

(†: Equal contributions)

1. **Bang, D.**, Lim, S., Lee, S., & Kim, S. (2023). Biomedical knowledge graph learning for drug repurposing by extending guilt-by-association to multiple layers. *Nature Communications*.

   - Contributions: Design and implementation of semantic teleport-based random walk for learning biomedical knowledge graph and case studies.

2. **Bang, D.**†, Koo, B.†, & Kim, S. (2024). Transfer learning of condition-specific perturbation in gene interactions improves drug response prediction. *Bioinformatics*–Transferred from *ISMB2024*

   - Contributions: Design and implementation of transfer learning pipeline between perturbational scales (gene to cell) and the condition-specific gene-gene attention.

3. Kim, Y.†, **Bang, D.**†, Koo, B., Yi, J., Cho, C., Choi, J., & Kim, S. (2025). MixingDTA: Improved Drug-Target Affinity Prediction by Extending Mixup with Guilt-By-Association. *ISMB/ECCB 2025* (Accepted)

   - Contributions: Design of LLM integration, Guilt-by-association based Mixup and case studies. Leading lab juniors for experimental setup.

4. **Bang, D.**, Sung, I., Piao, Y., Lee, S., & Kim, S. (2025). Predicting Drug-likeness via Biomedical Knowledge Alignment and EM-like One-Class Boundary Optimization. *ICML 2025* (Accepted for poster presentation)

   - Contributions: design and implementation of multi-modal alignment and EM-like optimization of drug-likeness boundary and case studies.

5. Lee, J.†, **Bang, D.**†, & Kim, S. (2024). Residue-Level Multiview Deep Learning for ATP Binding Site Prediction and Applications in Kinase Inhibitors. *Journal of Chemical Information and Modeling*, 65(1), 50-61.

   - Contributions: design of protein LLM with 3D geometric GNN integration, and kinase case studies, leading intern for experimental setup.

Awards, Honors & Grants

2023–2024	**Research Grant**: Advanced Medical Researcher Training Support Program (*Seoul National University*), Project Title: *Predicting Patient Drug Response with AI Using Transfer Learning and Omics Data*
Nov. 2024	**Best Paper Award**, Annual Conference of Korean Society for Bioinformatics (BIOINFO) 2024, Gyeongju, Republic of Korea
Nov. 2023	**Best Paper Award**, Annual Conference of Korean Society for Bioinformatics (BIOINFO) 2023, Yeosu, Republic of Korea
Aug. 2022	**Honnorable Mention** at The AI Korea 2022 poster presentation, KIISE Artificial Intelligence Society, Republic of Korea

Jul. 2022 **Honnorable Mention** at MOGAM Artificial Intelligence Symposium poster presentation, MOGAM Institute for Biomedical Research, Republic of Korea

Jun. 2022 **Grand Prize in Artificial Intelligence**, Korea Computer Congress (KCC) 2022, Jeju, Republic of Korea (Top 1/391 papers)

Presentations

Apr. 2025 **Poster Presentation**, Predicting Drug-likeness via Biomedical Knowledge Alignment and EM-like One-Class Boundary Optimization. *ICLR 2025 Workshop on Machine Learning for Genomics Explorations (MLGenX), Singapore*

Jul. 2024 **Oral Presentation**, Transfer learning of condition-specific perturbation in gene interactions improves drug response prediction. *International Conference on Intelligent Systems for Molecular Biology (ISMB) 2024, Montréal, Canada*

Jul. 2024 **Invited Talk**, Transfer learning of condition-specific perturbation in gene interactions improves drug response prediction. *Drug Discovery AI Workshop, Korea Computer Congress (KCC) 2024, Jeju, Republic of Korea*

Nov. 2023 **Guest Lecturer**, Introduction to Cheminformatics and databases & Network representation learning with word2vec. *AI-BIO Researcher Training Course, Artificial Intelligence Institute (AIIS), Seoul National University*

Nov. 2023 **Oral Presentation**, Biomedical knowledge graph learning for drug repurposing by extending guilt-by-association to multiple layers. *Annual Conference of Korean Society for Bioinformatics (BIOINFO) 2023, Yeosu, Republic of Korea*

Jul. 2023 **Invited Talk**, Biomedical knowledge graph learning for drug repurposing by extending guilt-by-association to multiple layers. *Biological Research Information Center (BRIC), POSTECH*

Nov. 2022 **Guest Lecturer**, Disease networks and drug repurposing. *AI-BIO Researcher Training Course, Artificial Intelligence Institute (AIIS), Seoul National University*

Teaching & Mentorship

Teaching (Computer Science & Engineering Dept., Seoul National University)

Spring 2025 **Teaching Assistant**, Machine Learning on Bioinformatics (English Lecture)
- Bioinformatics, Data & Machine Learning Algorithms for Cancer Classification
- Multi-Layer Perceptron and Deep Learning with PyTorch and CoLab

Fall 2024 **Teaching Assistant**, Algorithms
- Efficient string matching for whole-genome k-mer counting and sorting

Spring 2024 **Teaching Assistant**, Machine Learning on Bioinformatics (English Lecture)
- Bioinformatics, Data & Machine Learning Algorithms for Cancer Classification
- Multi-Layer Perceptron and Deep Learning with PyTorch and CoLab

Fall 2023 **Teaching Assistant**, Computer Convergence & Applications (English Lecture)
- Introduction to AI drug discovery: Navigating the chemical space with AI technologies

Spring 2023 **Teaching Assistant**, Machine Learning on Bioinformatics (English Lecture)
- Practical implementation of HMM for exon identification with Python
- Molecule representation learning & property prediction with Deep Learning

Spring 2022 **Teaching Assistant**, Machine Learning on Bioinformatics (English Lecture)
- Practical implementation of HMM for exon identification with Python

Mentorship

Spring 2025 **Team Mentor:** Development of RAG-Based AI Tool Selection and Interaction Platform for Drug Discovery, *Creative & Integrative Design Internship Course*

Fall 2024 **Team Mentor:** Real-time Ensemble Framework for Compound Activity Prediction from User Data Input, *Creative & Integrative Design Internship Course*

Spring 2024 **Team Mentor:** Integrating ADME data through multi-task learning for defining drug-likeness 2, *Creative & Integrative Design Internship Course*
– Resulted in publication at *ISMB/ECCB 2025.*

Winter 2023 **Mentor:** Biological Prior Knowledge-integrated Pocket-based Drug Design, *Research Internship Program for Interdisciplinary Major in Artificial Intelligence*

Fall 2023 **Team Mentor:** Integrating ADME data through multi-task learning for defining drug-likeness 1, *Creative & Integrative Design Internship Course*

Spring 2023 **Team Mentor:** ATP-binding site prediction using protein Language Models and 3D structure, *Creative & Integrative Design Internship Course*
– Resulted in publication at *Journal of Chemical Information and Modeling.*

Winter 2022 **Mentor:** Contrastive Learning Strategies for Molecular Property Prediction, *Research Internship Program for Interdisciplinary Major in Artificial Intelligence*

Fall 2022 **Team Mentor:** ATP-binding site prediction using 3D structure, *Creative & Integrative Design Internship Course*

Community Service

2022-2025 **Reviewer Involvement**
(Conferences) *AAAI, ICML, ICLR, KDD.*
(Journal) *Nature Communications, Nature Machine Intelligence, Nature Biomedical Engineering, Briefings in Bioinformatics, Bioinformatics, Scientific Reports.*

Technical Expertise

Machine Learning: PyTorch, PyTorch Geometric, HuggingFace Transformers, basic TensorFlow; Python-implemented machine learning algorithms and AutoML.
Bioinformatics & cheminformatics: RDKit, Biopython, DeepChem, TorchDrug, scanpy, basic R/Bioconductor
Data analysis & visualization: pandas, NumPy, anndata, seaborn, matplotlib

Last updated: July 3, 2025

Appendix

Full Publications List (†: Equal contributions)

Statistics: 11 Journal Publications (5 first/co-firsts), 5 Conference Proceedings (4 first/co-firsts), 3 Under Review (1 first) since 2022, with ∼150 citations (provided by Google Scholar).

Journal Publications

1. Kong, D.†, Ha, Y.†, Yoo, H.†, **Bang, D.**, & Kim, S. (2025). Survey on AI-Drug Discovery with Knowledge Graphs: Data, Algorithm and Application. *Journal of Computing Science and Engineering* (Accepted)
2. Ha, S.†, **Bang, D.**†, & Kim, S. (2025). FATE-Tox: Fragment Attention Transformer for E(3)-Equivariant Multi-Organ Toxicity Prediction. *Journal of Cheminformatics*, 17, 74.
3. Sung, I., Lee, S., **Bang, D.**, Yi, J., Lee, S., & Kim, S. (2025). MDTR: a knowledge-guided interpretable representation for quantifying liver toxicity at transcriptomic level. *Frontiers in Pharmacology*, 15, 1398370.
4. Lee, J.†, **Bang, D.**†, & Kim, S. (2024). Residue-Level Multiview Deep Learning for ATP Binding Site Prediction and Applications in Kinase Inhibitors. *Journal of Chemical Information and Modeling*, 65(1), 50-61.
5. Cho, C.†, Lee, S.†, **Bang, D.**, Piao, Y., & Kim, S. (2024). ChemAP: predicting drug approval with chemical structures before clinical trial phase by leveraging multi-modal embedding space and knowledge distillation. *Scientific Reports*, 14(1), 23010.
6. Pak, M., **Bang, D.**, Sung, I., Kim, S., & Lee, S. (2024). DGDRP: drug-specific gene selection for drug response prediction via re-ranking through propagating and learning biological network. *Frontiers in Genetics*, 15, 1441558.
7. Gu, J.†, **Bang, D.**†, Yi, J.†, Lee, S., Kim, D. K., & Kim, S. (2023). A model-agnostic framework to enhance knowledge graph-based drug combination prediction with drug–drug interaction data and supervised contrastive learning. *Briefings in Bioinformatics*, 24(5), bbad285.
8. **Bang, D.**, Lim, S., Lee, S., & Kim, S. (2023). Biomedical knowledge graph learning for drug repurposing by extending guilt-by-association to multiple layers. *Nature Communications*, 14(1), 3570.
9. Shin, J.†, Piao, Y.†, **Bang, D.**, Kim, S., & Jo, K. (2022). DRPreter: interpretable anticancer drug response prediction using knowledge-guided graph neural networks and transformer. *International Journal of Molecular Sciences*, 23(22), 13919.
10. **Bang, D.**†, Gu, J.†, Park, J., Jeong, D., Koo, B., Yi, J., ... & Lee, S. (2022). A survey on computational methods for investigation on ncRNA-disease association through the mode of action perspective. *International Journal of Molecular Sciences*, 23(19), 11498.
11. Lim, S.†, Lee, S.†, Piao, Y., Choi, M., **Bang, D.**, Gu, J., & Kim, S. (2022). On modeling and utilizing chemical compound information with deep learning technologies: A task-oriented approach. *Computational and structural biotechnology journal*, 20, 4288-4304.

Conference Proceedings

1. **Bang, D.**, Sung, I., Piao, Y., Lee, S., & Kim, S. (2025). Predicting Drug-likeness via Biomedical Knowledge Alignment and EM-like One-Class Boundary Optimization. *ICML 2025* (Accepted for poster presentation)
2. **Bang, D.**†, Kim, J.†, Song, H., & Kim, S. (2025). ADME-Drug-Likeness: Enriching Molecular Foundation Models via Pharmacokinetics-Guided Multi-Task Learning for Drug-likeness Prediction. *ISMB/ECCB 2025* (Accepted)

3. Kim, Y.†, **Bang, D.**†, Koo, B., Yi, J., Cho, C., Choi, J., & Kim, S. (2025). MixingDTA: Improved Drug-Target Affinity Prediction by Extending Mixup with Guilt-By-Association. *ISMB/ECCB 2025* (Accepted)
4. **Bang, D.**†, Koo, B.†, & Kim, S. (2024, July). Transfer learning of condition-specific perturbation in gene interactions improves drug response prediction. *ISMB2024* – Transferred to *Bioinformatics*, 40(Supplement_1), i130-i139.
5. Lee, D., Lee, D., **Bang, D.**, & Kim, S. (2024, March). DISCO: Diffusion schrödinger bridge for molecular conformer optimization. In *Proceedings of the AAAI Conference on Artificial Intelligence* (Vol. 38, No. 12, pp. 13365-13373).

Preprints and Under Review

1. Sung, I., **Bang, D.**, Kim, S., & Lee, S. Transferring Preclinical Drug Response to Patient via Tumor Heterogeneity-Aware Alignment and Perturbation Modeling. In *ICLR 2025 Workshop on Machine Learning for Genomics Explorations*
2. **Bang, D.**, Sung, I., & Kim, S. Predicting Therapeutic Outcome via Aligning Patient-Specific Knowledge Graphs and Translating Gene-Level Perturbation Patterns. (Under review)
3. Song, H., **Bang, D.**, & Kim, S. Network-Based Drug Recommendation via Biomedical Language Model-Enhanced Subgraph Embeddings (Under Review)