

Yoshitaka Inoue

Ph.D. Candidate in Computer Science · NIH Predoctoral Fellow
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Education

Ph.D. Candidate in Computer Science and Engineering, University of Minnesota, Twin Cities, USA 2021 – Present

Advisor: Prof. Rui Kuang; Co-advisor: Dr. Augustin Luna (NIH)

Expected graduation: August 2027

M.Eng. in Information Science, Nara Institute of Science and Technology, Japan 2017 – 2019

Advisor: Prof. Shigehiko Kanaya

B.Sc. in Biological Science, Kumamoto University, Japan 2012 – 2017

Advisor: Prof. Susumu Takio

Research Interests

- Machine learning for biological perturbations and therapeutic response
- Single-cell and functional genomics
- Intervention-aware representation learning
- Graph-based biomedical reasoning and LLM-based scientific reasoning

Research Experience

Pre-doctoral Fellow, National Library of Medicine / National Cancer Institute, NIH 2024 – Present

Co-advisor: Dr. Augustin Luna

- Develop machine learning methods for biological perturbation modeling and therapeutic response prediction across single-cell, pharmacogenomic, high-throughput screening, cancer cell-line, and patient datasets.
- Build treatment-conditioned latent-state transition models for transferring perturbation-response information to patient drug-response prediction.
- Develop graph-based drug-response models and biomedical reasoning systems that integrate molecular, pharmacologic, and clinical evidence.

Google Summer of Code Contributor; Mentor, Google Summer of Code 2022 – 2024

- Built a drug-response prediction pipeline and mentored projects on PyTorch Geometric datasets and multi-tool LLM aggregation for biomedical analysis.

Machine Learning Engineer, FreakOut, Inc., Tokyo, Japan 2019 – 2021

- Applied machine learning to click-through-rate prediction.

Peer-Reviewed Publications

Inoue, Y., Lee, H., Fu, T., Kuang, R., & Luna, A. (2026). drGT: Attention-Guided Gene Assessment of Drug Response Utilizing a Drug-Cell-Gene Heterogeneous Network. *BMC Bioinformatics*.

Inoue, Y., Hao, N., Lu, Y., Fu, T., & Luna, A. (2026). Drug Discovery in the Era of Artificial Intelligence: From Target Identification to Clinical Trials. *Health Data Science*.

Hoshi-Kadonosawa, Y., Reinhold, W. C., Taniyama, D., **Inoue, Y.**, et al. (2026). TRPM4 Expression as a Predictive Biomarker and a Mechanistic Driver of Acetalax Activity in Prostate Cancer: Preclinical Efficacy Studies. *Molecular Cancer Therapeutics*.

Elloumi, F., Reinhold, W. C., Varma, S., Wang, Y., Kinali, M., Arakawa, Y., **Inoue, Y.**, et al. (2026). CellMiner cross-database (CellMinerCDB) version 2.2 for explorations of patient-derived cancer cell line pharmacogenomics. *Nucleic Acids Research*.

Preprints and Manuscripts Under Review

Inoue, Y., Jeong, M., Hero, A., Kuang, R., & Luna, A. (2026). PerturbRx: Learning Treatment-Conditioned Latent Transitions for Patient Drug Response Prediction. *arXiv*.

Inoue, Y., Song, T., Wang, X., Luna, A., & Fu, T. (2026). DrugAgent: Reliable Multi-Agent Aggregation under Conflicting Biomedical Evidence. *Scientific Reports*. Under revision.

Taniyama, D., **Inoue, Y.**, Elloumi, F., Kim, Y. S., et al. (2026). Dynamic Schlafen 11 (SLFN11) expression revealed by single-cell RNA sequencing of clonal human cancer cells. *PLOS ONE*. Submitted.

Inoue, Y. (2024). scVGAE: A Novel Approach Using ZINB-Based Variational Graph Autoencoder for Single-Cell RNA-seq Imputation. *arXiv*.

Inoue, Y., Kulman, E., & Kuang, R. (2024). BiGCN: Leveraging Cell and Gene Similarities for Single-cell Transcriptome Imputation with Bi-Graph Convolutional Networks. *bioRxiv*.

Conference and Workshop Papers

Inoue, Y., Jeong, M., Hero, A., Kuang, R., & Luna, A. (2026). PerturbRx: Learning Treatment-Conditioned Latent Transitions for Patient Drug Response Prediction. *NeurIPS Workshop on World Models for High-Stakes Health (WMHS)*. Accepted (Poster).

Inoue, Y., Song, T., Wang, X., Luna, A., & Fu, T. (2026). DrugAgent: Reliable Multi-Agent Aggregation under Conflicting Biomedical Evidence. *ICML Workshop on Foundation Models for the Life Sciences (FM4LS)*.

Inoue, Y., Fu, T., & Luna, A. (2025). GraphPINE: Graph Importance Propagation for Interpretable Drug Response Prediction. *ICLR Workshop on Machine Learning for Genomics Explorations (MLGenX)*.

Inoue, Y., Song, T., Wang, X., Luna, A., & Fu, T. (2025). DrugAgent: Explainable Drug Repurposing Agent with Large Language Model-based Reasoning. *ICLR Workshop on Machine Learning for Genomics Explorations (MLGenX)*.

Selected Conference Presentations

Inoue, Y. (2026). PerturbRx: Learning Treatment-Conditioned Latent Transitions for Patient Drug Response Prediction [Poster presentation]. *New England Computational Biology Symposium (NECB)*, Boston, MA.

Inoue, Y. (2026). drGT [Oral presentation]. *ISMB Network Biology (NetBio) Community of Special Interest*, Washington, DC.

Inoue, Y. (2026). DrugAgent [Oral presentation]. *ISMB Text Mining Community of Special Interest*, Washington, DC.

Inoue, Y. (2026). drGT [Oral presentation]. *26th Annual CCR-FYI Colloquium*, Rockville, MD. Selected as one of four Outstanding Postgraduate Fellow Finalists.

Inoue, Y. (2025). drGT: attention-guided gene assessment for drug-response modeling [Oral presentation]. *NIH Artificial Intelligence Symposium*, Rockville, MD. Selected among 5 of 78 listed abstracts.

Fellowships, Awards, and Honours

NIH Predoctoral Research Fellowship 2024–Present

Outstanding Postgraduate Fellow Finalist, 26th Annual CCR-FYI Colloquium — selected as 1 of 4 finalists 2026

Research Visit Scholarships, NAIST and JASSO support for UC Davis research visits 2018–2019

Academic Service

Journal reviewing: BMJ Digital Health & AI (Expert Peer Reviewer, 2026–2027); IEEE/ACM Transactions on Computational Biology and Bioinformatics (2025–2027); Nature Computational Science (co-reviewer, 2026).

Conference reviewing: ACM BCB (2023); ICML FM4LS (2026); ICML GenBio (2026); IEEE BIBM (2026); ACM SIGSPATIAL (2026).

Technical Skills

Machine Learning / AI: Graph neural networks and heterogeneous graphs; autoencoders and latent-state models; representation learning; domain adaptation and transfer learning; treatment-conditioned transition modeling; LLM-based agents and retrieval-augmented generation; interpretable machine learning.

Computational Biology: Single-cell and bulk RNA-seq; pharmacogenomics and drug-response modeling; perturbation and functional genomics; cancer genomics; biological network analysis; multi-omics integration; biomedical knowledge graphs.

Frameworks: PyTorch; PyTorch Geometric; scikit-learn; LangChain; AutoGen.

Computational Infrastructure: Slurm; HPC; GPU computing; CUDA; Docker; uv; Ollama; LightLLM.

Last updated: September 30, 2026