

Yoshitaka Inoue

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Maryland, US | [GitHub](#) | [Google Scholar](#) | [LinkedIn](#)

Research Interests

Machine learning for molecular medicine; graph neural networks; drug response prediction; single-cell and perturbation modeling; intervention-aware representation learning; LLM-based biomedical reasoning.

Education

- 2021 - Present **University of Minnesota, Twin Cities**, Computer Science and Engineering, MN, US
Ph.D. candidate in Computer Science. Advisor: Prof. Rui Kuang. Co-advisor: Dr. Augustin Luna (NIH). Expected graduation: **September 2027**
- 2017 - 2019 **Nara Institute of Science and Technology**, Div. of Information Science, Nara, Japan M.Eng. in Information Science. Advisor: Prof. Shigehiko Kanaya
- Summer 2018 **University of California, Davis**, Genome Center, and DataLab, CA, US
Visiting Scholar. Advisors: Prof. Oliver Fiehn & Tobias Kind
- 2012 - 2017 **Kumamoto University**, Faculty of Science, Kumamoto, Japan, B.Sc. in Biological Science.
Advisor: Prof. Susumu Takio

Work Experience

- 2024 - Present **National Library of Medicine/National Cancer Institute**, MD, US
Pre-doctoral Fellow. Developing graph neural network and multi-agent AI frameworks for drug response prediction, drug-target reasoning, and biomedical evidence integration using pharmacogenomic, single-cell, HTS, cancer cell line, and patient datasets.
- Summer 2024 **Google Summer of Code**, Mentor
Mentored a project developing a large language model for multi-tool aggregation.
- Summer 2023 **Google Summer of Code**, Mentor
Mentored a project generating example datasets for PyTorch Geometric based on Pathway Commons.
- Summer 2022 **Google Summer of Code**, Contributor
Developed a pipeline for predicting drug response.
- 2019 - 2021 **FreakOut, Inc.**, Machine Learning Engineer, Tokyo, Japan
Applied machine learning to click-through rate prediction.

Publications

Peer-Reviewed Journal Articles

- 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.**, Luna, A., Kumar, S., Sun, N-Y., Kim, Y. S., Yin, J., Roper, N., Sowalsky, A. G., Figg, W. D., Takebe, N., & Pommier, Y. (2026) TRPM4 Expression as a Predictive Biomarker and a Mechanistic Driver of Acetalax Activity in Prostate Cancer: Preclinical Efficacy Studies. *Molecular Cancer Therapeutics*
- 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*
- Elloumi, F., Reinhold, W. C., Varma, S., Wang, Y., Kinali, M., Arakawa, Y., **Inoue, Y.**, Aladjem, M. I., Pommier, Y., & Luna, A. (2026). CellMiner cross-database (CellMinerCDB) version 2.2 for explorations of patient-derived cancer cell line pharmacogenomics. *Nucleic Acids Research*
- Murai, T., **Inoue, Y.**, Nambirige, A., & Annor, G. A. (2023). Machine learning approach in predicting GlutoPeak test parameters from image data with AutoML and transfer learning. *Heliyon*, 9(10), e20522.

Conferences

- Inoue, Y.**, Song, T., Wang, X., Luna, A., & Fu, T. (2026). DrugAgent: Reliable Multi-Agent Aggregation under Conflicting Biomedical Evidence. *ICML 2026 Workshop on FM4LS*
- Inoue, Y.**, Fu, T., & Luna, A. (2025). GraphPINE: Graph importance propagation for interpretable drug response prediction. *ICLR 2025 Workshop on MLGenX*
- Inoue, Y.**, Song, T., Wang, X., Luna, A., & Fu, T. (2025). DrugAgent: Explainable Drug Repurposing Agent

with Large Language Model-based Reasoning. *ICLR 2025 Workshop on MLGenX*

Preprints & Manuscripts Under Review

1. Taniyama, D., **Inoue, Y.**, Elloumi, F., Kim, Y. S., Rooper, N., Seibert, C., Kelly, M., Labanov, A., Aladjem, M. I., Luna, A., & Pommier, Y. (2026). Spontaneous dynamic gene expression of Schlafen 11 (SLFN11) demonstrated by single-cell RNA sequencing in clonal cancer cell lines. *PLOS ONE* (submitted)
2. **Inoue, Y.**, Song, T., Wang, X., Kuang, R., Fu, T., & Luna, A. (2026). DrugAgent: Reliable Multi-Agent Aggregation under Conflicting Biomedical Evidence. *Scientific Reports* (under revision), <https://arxiv.org/abs/2408.13378>
3. **Inoue, Y.** (2026). scVGAE: A ZINB-Based Variational Graph Autoencoder for Single-Cell RNA-Seq Imputation. *IEEE BIBM* (under revision), <https://arxiv.org/abs/2403.08959>
4. **Inoue, Y.**, Sun, S., Zhu, Q., & Luna, A. (2026). Integrating High-Throughput Screening and Biological Annotations for Machine-Learning-Based Therapeutic Candidate Prioritization in Glioblastoma. *IEEE BIBM* (under revision).
5. Xu, B., Lu, Y., **Inoue, Y.**, Lee, N., Fu, T., & Chen, J. (2024). Protein-Mamba: Biological Mamba Models for Protein Function Prediction. *arXiv preprint arXiv:2409.14617*, <https://arxiv.org/abs/2409.14617>
6. **Inoue, Y.**, Kulman, E., & Kuang, R. (2024). BiGCN: Leveraging Cell and Gene Similarities for Single-cell Transcriptome Imputation with Bi-Graph Convolutional Networks. *bioRxiv*, <https://doi.org/10.1101/2024.04.05.588342>

Oral Presentations

1. **Inoue, Y.**, Lee, H., Fu, T., Kuang, R., & Luna, A. drGT: Attention-Guided Gene Assessment of Drug Response Utilizing a Drug-Cell-Gene Heterogeneous Network, Accepted oral presentation, *34th Intelligent Systems for Molecular Biology (ISMB)*, Washington DC, US, July 12-16, 2026 (COSI: **Net Bio, 10 min**; also Student Council Symposium 15 min)
2. **Inoue, Y.**, Song, T., Wang, X., Luna, A., & Fu, T. DrugAgent: Explainable Drug Repurposing Agent with Large Language Model-based Reasoning. Accepted oral presentation, *34th Intelligent Systems for Molecular Biology (ISMB)*, Washington DC, US, July 12-16, 2026 (COSI: **Text Mining, 20 min**; also Student Council Symposium 15 min)
3. **Inoue, Y.**, Lee, H., Fu, T., Kuang, R., & Luna, A. drGT: Attention-Guided Gene Assessment of Drug Response Utilizing a Drug-Cell-Gene Heterogeneous Network, *26th Annual CCR-FYI Colloquium*, Rockville, MD, May 14-15, 2026 (**Selected as 1 of 4 Outstanding Postgraduate Fellow Finalists; 4/125 listed abstracts**)
4. **Inoue, Y.**, Lee, H., Fu, T., Kuang, R., & Luna, A. drGT: Attention-Guided Gene Assessment of Drug Response Utilizing a Drug-Cell-Gene Heterogeneous Network, *NIH Artificial Intelligence Symposium 2025*, Rockville, MD, May 16, 2025 (**5/78 listed abstracts**)

Poster Presentations

1. **Inoue, Y.** DrugAgent: Explainable Multi-Agent Reasoning for Aggregating Heterogeneous Biomedical Evidence. Poster presented at: *Deep Learning for Science Summer School (DL4Sci 2026)*; July 21, 2026; Berkeley, CA.
2. **Inoue, Y.**, Song, T., Wang, X., Luna, A., & Fu, T. DrugAgent: Reliable Multi-Agent Aggregation under Conflicting Biomedical Evidence. Poster presented at: *ICML 2026 Workshop on Foundation Models and Large Language Models for Life Sciences (FM4LS)*, Seoul, South Korea, July 2026.
3. **Inoue, Y.**, Lee, H., Fu, T., Kuang, R., & Luna, A. drGT: Attention-Guided Gene Assessment of Drug Response Utilizing a Drug-Cell-Gene Heterogeneous Network. Poster presented at: *AACR Annual Meeting 2026, Section 18, Board 7 (Abstract #7848)*; April 20, 2026; San Diego, CA.
4. **Inoue, Y.**, Fu, T., & Luna, A. GraphPINE: Graph importance propagation for interpretable drug response prediction. Poster presented at: *ICLR 2025 Workshop on Machine Learning for Genomics Explorations (MLGenX)*, Singapore, April 2025.
5. **Inoue, Y.**, Song, T., Wang, X., Luna, A., & Fu, T. DrugAgent: Explainable Drug Repurposing Agent with Large Language Model-based Reasoning. Poster presented at: *ICLR 2025 Workshop on Machine Learning for Genomics Explorations (MLGenX)*, Singapore, April 2025.

Technical Skills

- * ML/AI: Graph neural networks, graph representation learning, LLM-based agents, interpretable machine learning
- * Computational Biology: Pharmacogenomics, biological networks, single-cell RNA-seq, multi-omics analysis
- * Programming: Python, PyTorch, PyTorch Geometric, scikit-learn, pandas, NumPy

* Tools/Infrastructure: Git, Linux, Jupyter, Slurm, GPU computing, HPC cluster environments, LangChain
* Data: TCGA patient data, multi-omics data, cell line screening data

Professional Activities

Journal Reviewing

- IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2025–2026
- Nature Computational Science, Co-reviewer, 2026
- Frontiers in Bioinformatics, 2026

Conference & Workshop Reviewing

- ACM BCB, 2023
- ICML Workshop on Foundation Models for the Life Sciences (FM4LS), 2026
- ICML Workshop on Generative Biology (GenBio), 2026
- IEEE BIBM, 2026
- ACM Sigspatial, 2026

Memberships

- International Society for Computational Biology (ISCB)
- American Association for Cancer Research (AACR)
- American Society of Clinical Oncology (ASCO)

Honors & Fellowships

2024–Present	NIH Pre-Doctoral Research Fellowship
Feb 2019	NAIST Research Visit Scholarship, UC Davis
Jun–Sep 2018	NAIST Research Visit Scholarship, UC Davis
Jun–Sep 2018	JASSO Research Visit Scholarship, UC Davis