Curriculum Vitae

Kairi Furui

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Department of Computer Science, School of Computing, Institute of Science Tokyo

Current Status: Ph.D. student, JSPS DC1 Research Fellow, ACT-X Researcher

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Date of Birth: 4 April 1999
Place of Birth: Tochigi, Japan
Citizenship: Japan

Education:

Present	Ph.D. student, Department of Computer Science, School of Computing, Institute of Science Tokyo, Kanagawa, Japan. (Expected: March 2027)
2024	M.Sc., Eng., Department of Computer Science, School of Computing, Tokyo Institute of Technology, Kanagawa, Japan.
2022	B.Sc., Eng., Department of Computer Science, School of Computing, Tokyo Institute of Technology, Japan.
2020	Semi. B.Sc., Eng., Department of Innovative Electrical and Electronic Engineering, National Institute of Technology, Oyama College, Japan.

Current Research Interests:

Bioinformatics, Cheminformatics, Computational Chemistry, Machine Learning, Free Energy Perturbation, Antibody Design

Publications Peer-reviewed:

1. Masunaga S†, Furui K†, Kengkanna A, Ohue M. GraphBioisostere: general bioisostere prediction model with deep graph neural network J. Supercomput., 82.3, 132, 2026., 10.1007/s11227-026-08232-y

2. Ohue M, **Furui K** PBPredictor.net: GBDT-based model and web tool for prediction of blood–placental barrier permeability of small molecules J. Supercomput., 82.2, 93, 2026., 10.1007/s11227-026-08233-x

3. **Furui K**, and Ohue M. Boltzina: Efficient and Accurate Virtual Screening via Docking-Guided Binding Prediction with Boltz-2. AI for Accelerated Materials Design Workshop at the 39th Conference on Neural Information Processing Systems (AI4Mat workshop on NeurIPS2025), 2025

4. **Furui K**, and Ohue M. ALLM-Ab: Active Learning-driven antibody optimization using fine-tuned protein Language Models. J. Chem. Inf. Model., 65.21, 11543-11557, 2025., 10.1021/acs.jcim.5c01577

5. **Furui K**, Sakano K, Ohue M. Predictive and therapeutic applications of protein language models. Allergol. Int., 74.4, 534-548, 2025., 10.1016/j.alit.2025.08.004

6. Uchikawa K, **Furui K**, and Ohue M. Leveraging AlphaFold2 Structural Space Exploration for Generating Drug Target Structures in Structure-Based Virtual Screening Biochem. Biophy. Rep., 43, 102110, 2025., 10.1016/j.bbrep.2025.102110

7. Masunaga S†, Furui K†, Kengkanna A, Ohue M. GraphBioisostere: General Bioisostere Prediction Model with Deep Graph Neural Network. In Proc PDPTA'25, IEEE CPS, 2025. †: equally contributed

8. Ohue M, **Furui K** GBDT-based Model and Web Tool for Prediction of Blood-Placental Barrier Permeability of Small Molecules. In Proc PDPTA'25, IEEE CPS, 2025

9. **Furui K**, and Ohue M. Benchmarking HelixFold3-Predicted Holo Structures for Relative Free Energy Perturbation Calculations ACS Omega., 10.11, 11411-11420, 2025., 10.1021/acsomega.4c11413

10. **Furui K**, Shimizu T, Akiyama Y, Kimura S R, Terada Y, and Ohue M. PairMap: An Intermediate Insertion Approach for Improving the Accuracy of Relative Free Energy Perturbation Calculations for Distant Compound Transformations J. Chem. Inf. Model., 65.2, 705–721, 2025., 10.1021/acs.jcim.4c01634

11. Sakano K, **Furui K**, Ohue M. NPGPT: natural product-like compound generation with GPT-based chemical language models J. Supercomput., 81.1, 1-16, 2025., 10.1007/s11227-024-06860-w

12. **Furui K**, and Ohue M. Active learning for energy-based antibody optimization and enhanced screening. Machine Learning in Structural Biology Workshop at the 38th Conference on Neural Information Processing Systems (MLSB workshop on NeurIPS2024), 2024

13. Sakano K, **Furui K**, Ohue M. Natural Product-like Compound Generation with Chemical Language Models. In Proc PDPTA'24, IEEE CPS, 2024

14. **Furui K**, Ohue M. Fastlomap: faster lead optimization mapper algorithm for large-scale relative free energy perturbation J. Supercomput., 80.10, 14417-14432, 2024., 10.1007/s11227-024-06006-y

15. Murakumo K, Yoshikawa N, Kentaro R, Nakamura S, **Furui K**, Suzuki T Yamasaki H, Nishigaya Y, Takagi Y & Ohue M. LLM Drug Discovery Challenge: A Contest as a Feasibility Study on the Utilization of Large Language Models in Medicinal Chemistry. AI for Accelerated Materials Design-NeurIPS 2023 Workshop, 2023

16. Ochiai T, Inukai T, Akiyama M, **Furui K**, Ohue M, Matsumori N, Inuki S, Uesugi M, Sunazuka T, Kikuchi K, Kakeya H & Sakakibara Y. Variational autoencoder-based chemical latent space for large molecular structures with 3D complexity. Commun. Chem., 6, 249, 2023., 10.1038/s42004-023-01054-6

17. **Furui K**, and Ohue M. Faster Lead Optimization Mapper Algorithm for Large-Scale Relative Free Energy Perturbation. In Proc PDPTA'23, IEEE CPS, 2023

18. **Furui K**, and Ohue M Compound Virtual Screening by Learning-to-Rank with Gradient Boosting Decision Tree and Enrichment-based Cumulative Gain. 2022 IEEE Conference on Computational Intelligence in Bioinformatics and Computational Biology (CIBCB), 2022

Grants and Scholarships:

- 2025/10-2028/3: ACT-X [Life and Information] [JPMJAX25LB], Japan Science and Technology Agency (JST), “Highly Accurate Free Energy Prediction for Multi-Point Mutation”
- 2024/4-2027/3: JSPS Research Fellow DC1 [24KJ1091], Japan Society for the Promotion of Science (JSPS), “Development of Drug Discovery Lead Optimization Methods Combining Deep Learning and Free Energy Perturbation Calculations”
- 2022/4-2024/3: JASSO Type 1 Scholarship Full Exemption for Outstanding Achievement [], Japan Student Services Organization (JASSO), “”

Awards:

- AHeDD2025 Wiley Best Poster Award (2nd Class) (2025)
- IPSJ SIGBIO Excellent Student Award (2023)
- 74th IPSJ SIGBIO Excellent Presentation Award (2023)
- 70th IPSJ SIGBIO Excellent Presentation Award (2022)
- Student Encouragement Award of 84th IPSJ National Convention (2022)
- IPSJ Steering Committee on Network Software Young Researcher Award (2019)
- Student Encouragement Award of 82nd IPSJ National Convention (2019)

Products:

- Boltzina (2025): ohuelab/boltzina
  Efficient virtual screening software combining Boltz-2 and AutoDock Vina
- ALLM-Ab (2025): ohuelab/ALLM-Ab
  Multi-objective antibody optimization using protein language models and active learning
- Anchored Docking Workflow (2024): YumizSui/anchored_docking_workflow
  Anchored docking preparation workflow for AutoDock
- PairMap (2024): ohuelab/PairMap
  Intermediate compound insertion method for relative free energy perturbation calculations
- FastLomap (2023): ohuelab/FastLomap
  Fast perturbation map construction method for large-scale relative free energy perturbation calculations
- PBPredictor (2021): pbpredictor.net/
  Web tool for predicting blood-placental barrier permeability

Skills:

- Programming Languages: Python, Shell, C++
- Machine Learning: Scikit-learn, PyTorch, DDP
- Cheminformatics & Bioinformatics: RDKit, Biopython, PyMOL
- High-Performance Computing: TSUBAME3.0, TSUBAME4.0
- Molecular Docking: AutoDock Vina, Glide
- Protein Structure Prediction: AlphaFold2, AlphaFold3, Boltz-2
- Free Energy Perturbation: Flare FEP, OpenFE
- Molecular Dynamics Simulation: Amber, GROMACS

Invited Talks (Japanese):

- 2025: FIT2025 Top Conference Session: Bioinformatics / Welfare Informatics / Computer Vision and Image Media - "Energy-Based Antibody Optimization and Active Learning for Antibody Screening"
- 2025: 15th CBI Young Researchers Meeting - Present and Future of Drug Discovery Research - "Multi-Objective Active Learning Using Protein Language Models for Efficient Antibody Optimization"
- 2023: Structure-Activity Forum 2023 - "#LLM Drug Discovery Challenge Report - A Feasibility Study on LLM Utilization in Drug Discovery" (Presented as a top winner of the #LLM Drug Discovery Challenge)

Internship (Japanese):

- 2023/8-2023/9: DeNA Summer Internship 2023 AI Specialist Course
- 2022/8-2022/9: Preferred Networks

Part-time Work:

- Ahead Biocomputing, Co. Ltd. 2023–

Collaborative Research:

- Astellas Pharma Inc. de novo antibody design (Research Assistant at Ohue Laboratory)
- Perseus Proteomics Inc. (Research Assistant at Ohue Laboratory) [Link]
- Alivexis, Inc. (Research Assistant at Ohue Laboratory) [Link]

Teaching (Japanese):

- 2025: AJACS: Learning and Using AlphaFold and Other Protein Structure Prediction Tools
- 2024: AI and Organic Synthetic Chemistry Study Group 14th Meeting - Cheminformatics Hands-on Workshop Instructor Support
- 2024: University of Tokyo, Graduate School of Engineering, Chemical Data Science Lecture
- 2021-2024: Tokyo Institute of Technology, School of Computing - Procedural Programming Fundamentals TA
- 2021-2024: Tokyo Institute of Technology, School of Computing - Advanced Procedural Programming TA

Peer Review:

- Journal of Chemical Information and Modeling (2025): 1 manuscript
- JACS Au (2025): 1 manuscript

Organization of Meetings (Japanese):

- 2024: 16th Annual Meeting of Young Researchers in Bioinformatics - Staff (Staff)
- 2022: (Staff)

Affiliated Societies (Japanese):

- Japanese Society for Bioinformatics
- Information Processing Society of Japan

Last updated: February 6, 2026