Session 1 13:05-13:45

Gearing up for the acceleration: From High-Fidelity Organ-on-Chip Systems to the Self-Driving Human Organ Mimicry Platform

Dr. Yimu Zhao

Acceleration Consortium, University of Toronto

Abstract

Human-derived organoid and organ-on-chip systems have emerged as essential tools for drug screening and disease modeling, addressing the limitations of animal models and oversimplified cell cultures that fail to capture human-specific genetic and physiological diversity. By reproducing the cellular architecture, mechanical microenvironment, and biochemical signaling of human tissues, these systems enable more clinically relevant predictions of therapeutic efficacy and toxicity.

Early efforts focused on simple co-culture models, combining primary functional cells with supporting population to demonstrate the organ-specific function, the contractility of the heart, as an example, is the main function of the heart, has been demonstrated in heart-on-a-chip platform to screen compounds for cardiotoxicity and therapeutic effect. To improve the model fidelity, vasculature with resident macrophages were introduced to the system to form dynamic cellular circuits, where resident macrophages support vascular stability and promote advance cardiac function. These advances highlight the necessary components to built clinically relevant microenvironment that could improve the physiological fidelity of tissues. However, these advances demonstrate the culture fidelity but also introduced new challenges: batch-to-batch variability, limited scalability, resource intensity, and reliance on highly specialized expertise.

To overcome these constraints, current efforts have focused on developing automation-compatible culture platforms that integrate embedded sensors, robotic handling of microscale droplets, and computer vision–based decision-making. The system supports automated seeding and longitudinal monitoring of cardiac microtissues and vascularized organ cultures-on-chip over multiweek periods, enabling stable long-term culture and analysis. These integrated systems allow precise fluid manipulation, continuous assessment of microenvironmental parameters, and intelligent adjustment of experimental conditions in response to real-time feedback. Coupled with machine learning algorithms, they enable data-driven optimization of tissue growth, differentiation, and function.

Collectively, these convergent technologies define the Self-Driving Human Organ Mimicry Platform, an autonomous framework that unites organoid and organ-on-chip engineering with AI-guided experimental control. This transition from manually operated organ-on-chip systems to a self-driving, sensor-rich, and data-intelligent platform establishes a new paradigm for adaptive modeling of human organ physiology and accelerates the translation of experimental biology into precision medicine.

Keyword

Organ-on-a-chip, self-driving lab, screening, tissue model, organoids

Short biography

Dr. Yimu Zhao is a Staff Scientist at the Acceleration Consortium, where she leads research in organoid and organ-on-a-chip technologies for modeling human physiology and disease. Her primary research interest lies inrecapitulating organ-specific microenvironments and promoting functional maturation through engineered multicellular systems.

Dr. Zhao completed her Ph.D. in Biomedical Engineering at the University of Toronto in 2019. During her doctoral studies, she designed and developed the Biowire II Organ-on-a-Chip platform, a drug-inert tissue culture and testing system that employs super-elastic biomaterials as biosensors to cultivate three-dimensional, adult-like cardiac tissue arrays. Integrating principles from developmental biology, tissue engineering, and microfluidics, this platform enables the generation of chamber-specific, healthy, and patient-derived cardiac tissues and provides continuous functional readouts through its material-based sensing system.

Following her Ph.D., Dr. Zhao's postdoctoral research focused on building organ-specific vascular networks and multi-organ systems for studying drug responses and disease phenotypes across diverse tissue types. Her translational work bridges basic biological discovery with pharmaceutical applications, emphasizing reproducibility, scalability, and integration with automation.

Dr. Zhao is also the co-founder of TARA Biosystems, a biotechnology company founded on the Biowire II technology and acquired by Valo Health in 2022. She has authored over 40 peer-reviewed publications and holds six patents, including a first-author paper published and highlighted in Cell.

Specialty and present interests

Tissue engineering, organ-on-a-chip, vascularized tissues, self-driving lab, high throughput/high content screening

References

1. Zhao, Y., et al., *Geometrically controlled cardiac microtissues promote vascularization and reduce inflammation in vitro and in vivo.* Cell Biomaterials, 2025. **1**(4).
2. Zhao, Y., et al., *Integrating organoids and organ-on-a-chip devices.* Nature Reviews Bioengineering, 2024. **2**(7): p. 588-608.
3. Zhao, Y., et al., *A Platform for Generation of Chamber-Specific Cardiac Tissues and Disease Modeling.* Cell, 2019. **176**(4): p. 913-927 e18.
4. Landau, S., et al., *Primitive macrophages enable long-term vascularization of human heart-on-a-chip platforms.* Cell Stem Cell, 2024. **31**(8): p. 1222-1238 e10.
5. Wu, Q., et al., *Automated fabrication of a scalable heart-on-a-chip device by 3D printing of thermoplastic elastomer nanocomposite and hot embossing.* Bioact Mater, 2024. **33**: p. 46-60.

Session 1　13:45-14:10

The Living Laboratory: Fully Automated Science Powered by AI Agents and Physical AI

Dr. Genki Kanda

Department of Robotic Science, Medical Research Laboratory, Institute of Science Tokyo

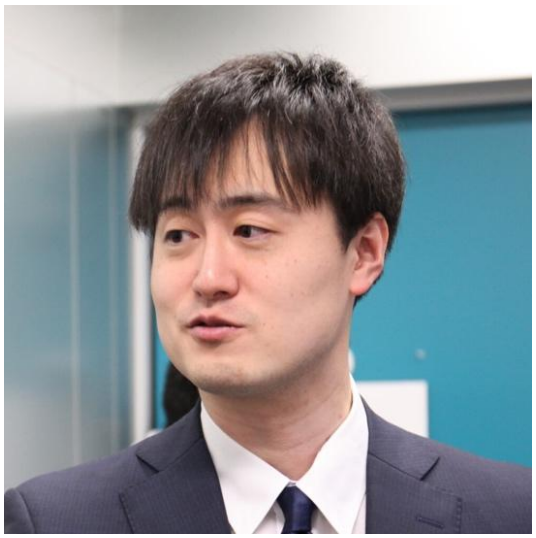
Abstract

omation across a wide range of laboratory procedures, while recent progress in artificial intelligence (AI) agents is laying the groundwork for autonomous reasoning combined with robotic execution, extending toward the generation of scientific papers without human intervention. However, fully automated science cannot be realized solely with cyber-space AI agents and robots executing human-specified protocols. In practice, substantial human "*Care*" remains indispensable for preparation, setup, and troubleshooting. We classified the *Care* into two types: Planning *Care* and Operation *Care*. Since a bottom-up attempt to automate every instance of *Care* is unbounded, we introduced self-maintainability as a top-down framework (Ochiai et al., *Digital Discovery*, 2025). Within this framework, Planning *Care* is assigned to AI agents, while Operation *Care* is assigned to physical AI, together forming what we call the Living Laboratory. In automating Planning *Care*, the main objective is to minimize the need for precise user instructions. Traditionally, users had to adapt protocols to the availability of instruments and consumables, but we developed multiple AI-based systems that handle this process autonomously. These systems can encode experimental protocols as deterministic finite automata for dynamic and loop-aware execution, translate natural language procedures into executable robotic programs through large language models (LLMs), and interpret the intentions of human users or AI scientists to generate structured experimental plans. By combining these complementary approaches, the system relieves operators from manual scheduling and configuration work and enables truly unmanned front-end operation in complex biological experiments. In automating Operation *Care*, the goal is to sustain experiments by adapting to the laboratory environment. We developed a vision-language model (VLM)-based operating system that autonomously executes implicit tasks such as tip attachment using visual information, ensures reliable operation by running programs in simulation and correcting detected errors through language models, and identifies user-induced inconsistencies such as mis-assigned deck positions to provide corrective suggestions. This system is integrated with robotic arms, functioning as a vision-language-action (VLA) model-based system. To consolidate these technologies, we are currently developing a centralized city-center robotic facility at the Institute of Science Tokyo, designed to integrate multiple experimental robots and VLA-enabled systems. Automation of *Care* represents the final barrier to achieving fully automated science, and the self-maintainability framework provides a systematic strategy for addressing *Care* tasks while preventing an endless accumulation of ad hoc solutions. The Living Laboratory establishes a scalable trajectory that begins at the bench level and extends to the room and eventually the floor level, outlining a roadmap for how automated facilities can evolve from individual workstations into comprehensive autonomous laboratories.

Keyword

Laboratory automation, Artificial intelligence agents, Self-maintainability, Living Laboratory,

Physical AI



Short biography

Dr. Kanda received his PhD in Science from Osaka University. After encountering the Maholo LabDroid in 2015, he began leading initiatives to develop and implement laboratory automation, demonstrating practical applications through regenerative medicine. In 2019, he founded the Laboratory Automation Supplier's Association (LASA) in Japan, where he continues to serve as chairman and actively promotes community engagement in laboratory automation. As of April 2025, he serves as a Professor at the Institute of Science Tokyo.

Specialty and present interests

Developing robotic and AI technologies that transform life science research from human-centered to collaborative approaches with robots and AI. Focusing on laboratory automation, AI agents, and embodied intelligence to advance efficiency, accuracy, and new methodologies in experimental research.

References

Yachie et al. Robotic Crowd Biology with Maholo LabDroids. *Nature Biotechnology* (2017).
Kanda and Tsuzuki et al. Autonomous Optimization for Cell Culture. *eLife* (2022).
Ochiai et al. Automating Care by Self-Maintainability for Full Laboratory Automation. *Digital Discovery* (2025).

Session 1　14:10-14:35

Machine Learning for Robots: From Perception to Action

Dr. Asako Kanezaki

Institute of Science Tokyo

Abstract

To build a robotic system that operates in real-world environments, it is necessary to recognize the environment and acquire policies that determine optimal actions based on the recognition results. In this talk, I will introduce the recent work of our laboratory in areas such as 3D object recognition, robot manipulation, multi-agent cooperative behavior learning, and research in the field of Embodied AI. In recent 3D object recognition research, category-level pose estimation for unseen objects has been actively studied. We proposed a self-supervised method for part-level pose estimation. In the field of robotic manipulation, we are working on dexterous object-handling tasks such as cable insertion. As part of our research on multi-robot cooperative behavior learning, we proposed a self-localization method using event cameras. Finally, in the field of Embodied AI, particularly in visual navigation tasks, we introduce new approaches such as navigation learning with action description as an auxiliary task, and an environment description task based on autonomous exploration.

Keyword

3D object recognition, robot visual navigation, robot manipulation, multiagent, machine learning

Short biography

ASAKO KANEZAKI received the B.S., M.S. and Ph.D. degrees in information science and technology from The University of Tokyo, in 2008, 2010, and 2013, respectively. In 2010, she was a Visiting

Researcher with the Intelligent Autonomous Systems Group, Technische Universität München. From 2013 to 2016, she was an Assistant Professor with The University of Tokyo. She was with the National Institute of Advanced Industrial Science and Technology (AIST), from 2016 to 2020. Since 2020, she has been an Associate Professor with the Institute of Science Tokyo (formerly, Tokyo Institute of Technology). She also joined RIKEN Center for Advanced Intelligence Project (AIP) as a team director in 2025. Her current research interests include 3D object recognition, semantic mapping, and robot applications, such as visual navigation and manipulation.

Specialty and present interests

3D object recognition, semantic mapping, and robot applications, such as visual navigation and manipulation.

References

[1] H. Kondoh and A. Kanezaki. Embodied navigation with auxiliary task of action description prediction. In *IEEE/CVF International Conference on Computer Vision (ICCV)*, 2025.

[2] M. Yajima, K. Ota, A. Kanezaki, and R. Kawakami. Zero-shot peg insertion: Identifying mating holes and estimating se(2) poses with vision-language models. In *IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*, 2025.

[3] K. Matsumoto and A. Kanezaki. Eed: Embodied environment description through robotic visual exploration. In *The 6th Embodied AI workshop at CVPR*, 2025.

[4] Y. Che, R. Furukawa, and A. Kanezaki. Op-align: Object-level and part-level alignment for self-supervised category-level articulated object pose estimation. In *The 18th European Conference on Computer Vision (ECCV)*, oral, 2024.

[5] H. Nakagawa, Y. Miyatani, and A. Kanezaki. Linking vision and multi-agent communication through visible light communication using event cameras. In *Int Joint Conf on Autonomous Agents & Multiagent Systems (AAMAS)*, 2024.

Session 1　14:35-15:00

Empowering Researchers with AI-Powered Automation

Dr. Kazue Mizuno

Preferred Networks, Inc.

Abstract

In the life sciences field, AI technologies are widely used for various applications including molecular design for drug discovery, protein structure prediction, disease diagnosis and prognosis prediction and omics data analysis. Furthermore, by combining image recognition technology with robotics, routine experimental tasks for both *in vitro* and *in vivo* experiments have been successfully automated. One of our laboratory automation products is AUTiv®, an automated intravenous drug administration system for mice released in 2024. This product not only reduces the burden of the researchers and technicians but also contributes to improved animal welfare, reducing researchers' stress while freeing up time for more creative research work. Another example is Kachaka®, an autonomous mobile robot used for repetitive tasks such as sample transfer and transport of contaminated equipment in laboratory and clinical settings.

The latest innovations in generation AI are dramatically expanding the possibilities for experimental automation. For instance, in recent research conducted by our company, incorporating foundation models enabled robust segmentation of transparent experimental equipment like glass containers, while novel mechanical designs facilitated delicate and adaptive handling of laboratory instruments by robots.

One of the key challenges in experimental automation for the life sciences field is accurately executing the entire cycle of hypothesis generation, experimental protocol preparation, data analysis, and subsequent hypothesis formulation based on results. While currently available LLMs (Large Language Models) can provide some assistance with these tasks, they still lack sufficient performance to reliably complete experiments. Looking ahead, we anticipate that generative AI technologies—including AI agents—when integrated with automated experimental equipment, will further accelerate the research and development cycle.

In this presentation, the research and development cases conducted by Preferred Networks regarding experimental automation in the life sciences field will be introduced.

Keyword

Robotics, Generative AI

References

1. https://www.summitpharma.co.jp/japanese/service/products/autiv/
2. https://kachaka.life/

3. Avinash Ummadisingu, Jongkeum Choi, Koki Yamane, Shimpei Masuda, Naoki Fukaya, Kuniyuki Takahashi, "**SAID-NeRF: Segmentation-AIDed NeRF for Depth Completion of Transparent Objects,**" IROS2024
4. Naoki Fukaya, Koki Yamane, Shimpei Masuda, Avinash Ummadisingu, Shin-ichi Maeda, Kuniyuki Takahashi: "**Four-Axis Adaptive Fingers Hand for Object Insertion: FAAF Hand**," IROS2024
5. Kuniyuki Takahashi, Shimpei Masuda, Tadahiro Taniguchi: "**Stable Object Placing using Curl and Diff Features of Vision-based Tactile Sensors,**" IROS2024

Session 2　15:30-16:10

The Cutting Edge of AI in the Healthcare and Life Sciences

Dr. Yurika Osuji

Google for Health

Abstract

Artificial intelligence (AI) stands as a transformative force in history, poised to revolutionize the natural sciences. This presentation explores the cutting edge of AI in healthcare and life sciences, tracing the journey from foundational breakthroughs to practical applications in discovery and care.

We begin with the legacy of AlphaGo, which demonstrated AI's capacity to master complex systems. This potential was realized in biology with AlphaFold, which solved the 50-year grand challenge of protein structure prediction. This breakthrough, recognized with the 2024 Nobel Prize in Chemistry, is now accelerating research into global challenges, from antibiotic resistance to plastic pollution. We discuss the evolution of this technology, including AlphaFold 3 for predicting broad protein-molecule interactions and AlphaMissense for classifying human genetic variants. Expanding into genomics, we introduce AlphaGenome, which models gene regulation by reading contexts of one million DNA letters, and Cell2Sentence, a foundation model for single-cell analysis that bridges cellular biology with language modeling.

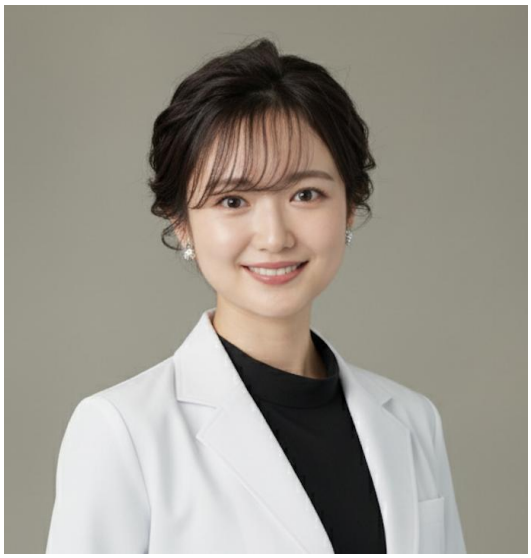
In the field of therapeutics, we examine how LLMs are accelerating drug discovery. We present TxGemma, a model fine-tuned for therapeutic tasks, and Agentic-Tx, a system that employs reasoning and tool use to navigate the complex drug development lifecycle.

Translating these advances to clinical settings, we discuss MedGemma, a family of open models for medical image and text comprehension. We also highlight AMIE (Articulate Medical Intelligence Explorer), a conversational diagnostic AI that has demonstrated expert-level diagnostic accuracy and high ratings for empathy in simulated clinical evaluations. Furthermore, we touch upon personal health innovations with SensorLM and the Personal Health Agent, which utilize multimodal wearable data to provide actionable wellness insights.

Finally, we introduce the AI co-scientist, a novel multi-agent system built on Gemini. By mimicking the scientific method—generating, debating, and refining hypotheses—this system represents a paradigm shift towards autonomous scientific discovery. Together, these technologies illustrate a future where AI acts as a partner in unraveling the mysteries of biology and improving human health.

Keyword

Artificial Intelligence, Healthcare, Life Sciences, Genomics, AI Co-scientist



Short biography

Specialty and present interests: Clinical Specialist, AI in Medicine. Present interests: Applying large-scale AI models to healthcare and life sciences, including genomics, therapeutics, clinical diagnostics, and accelerating foundational scientific research .

References

Jumper, J. et al. (2021). Highly accurate protein structure prediction with AlphaFold. Nature 596, 583–589.

Tu, T. et al. (2025). Towards conversational diagnostic artificial intelligence. Nature 642, 442-450.

Gottweis, J. et al. (2025). Towards an AI co-scientist.

Narayanswamy, G. et al. (2024). Scaling Sensor Data Modeling (SensorLM).

Chaves, JMZ. et al. (2024). Tx-LLM: A Large Language Model for Therapeutics.

Session 2　16:10-16:35

AI-Driven Insights into Protein Complexes and Dynamics

Dr. Ryuichiro Ishitani

Medical Research Laboratory, Institute of Science Tokyo

Abstract

Artificial intelligence has fundamentally transformed our ability to understand and engineer protein complexes and their dynamic behaviors. This talk presents an integrated framework of AI-driven methodologies that address key challenges across structural biology, from accurate complex prediction to dynamic sampling and rational protein design.

We develop restraint-guided inference methods that extend AlphaFold3's diffusion model capabilities in multiple directions. First, by applying stereochemical restraints during reverse diffusion, we eliminate chirality errors and improve ligand geometries in protein-ligand complexes, enhancing structure-based drug discovery applications. Second, by implementing distance restraints between atomic groups, we efficiently sample conformational changes and ligand binding/dissociation pathways along specified reaction coordinates. Integration with molecular dynamics simulations enables quantitative free energy landscape calculations, successfully reproducing experimental thermodynamics for protein conformational transitions and protein-ligand binding processes.

Beyond individual complexes, we demonstrate the power of AI for systems-level understanding through high-throughput prediction of protein-protein interactions in biosynthetic gene clusters. Systematic screening of nearly 500,000 protein pairs from 2,437 BGCs reveals thousands of previously uncharacterized interactions, illuminating hidden molecular mechanisms in natural product biosynthesis.

Finally, we extend AI's utility to protein design by combining ProteinMPNN with multi-objective optimization algorithms, generating structurally similar proteins with remarkable sequence diversity—achieving less than 10% sequence identity while maintaining target fold architecture.

Together, these AI-driven approaches demonstrate how advanced computational methods can illuminate protein structure, dynamics, interactions, and design, establishing new paradigms for understanding and engineering biological systems.

Keyword

Structure prediction, Drug design, Conformational sampling, Protein design

Short biography

Ryuichiro Ishitani has held academic positions at leading Japanese institutions since 2003. They served as Associate Professor at the University of Tokyo's Institute of Medical Science (2008-2010) and the Graduate School of Science (2010-2018). In 2018, they joined Preferred Networks, Inc. as an Engineering Manager while concurrently serving as Project Professor at the University of Tokyo.

Since January 2024, they have been Professor at Tokyo Medical and Dental University's Medical Research Institute, and currently at the Institute of Science Tokyo's Institute of Integrated Research, Medical Research Institute following the institutional merger in October 2024.

Specialty and present interests

Application of deep learning to structural biology and drug discovery

References

Yoshitaka Moriwaki, Taro Shiraishi, Yohei Katsuyama, Kenichi Matsuda, Toyoyuki Ose, Atsushi Minami, Hideaki Oikawa, Tomohisa Kuzuyama, Ryuichiro Ishitani, Tohru Terada Predicting protein complexes in biosynthetic gene clusters, bioRxiv, DOI:10.1101/2025.10.26.684697, (2025).

Ryo Akiba, Yoshitaka Moriwaki, Ryuichiro Ishitani, Naruki Yoshikawa, Multi-objective optimization for designing structurally similar proteins with diverse sequences, bioRxiv, DOI:10.1101/2025.09.13.676063, (2025).

Ryuichiro Ishitani, Yoshitaka Moriwaki, Improving Stereochemical Limitations in Protein-Ligand Complex Structure Prediction, ACS Omega, DOI: 10.1021/acsomega.5c07675, (2025).

Session 2　16:35-17:00

Closed-loop Protein Design with Generative AI and Molecular Dynamics

Dr. Shuto Hayashi

Medical Research Laboratory, Institute of Science Tokyo

Abstract

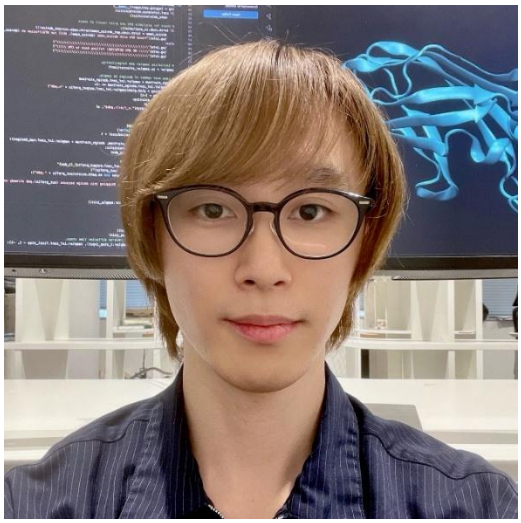
In recent years, protein (and also peptide) design using generative AI has attracted significant attention. However, success rates remain suboptimal, largely due to the vast sequence search space and the insufficient utilization of experimental evaluation data. Thus, there is a critical need for design strategies that can efficiently navigate this space and leverage feedback from functional evaluations. To address these challenges, we developed an autonomous design loop that integrates AI-based protein generation, simulation-based and experimental functional evaluation, and Bayesian optimization for iterative feedback. This platform systematically evaluates whether generated proteins exhibit the desired functionality and identifies key factors that distinguish functional from non-functional proteins. These insights are then fed back into the generative AI to guide more focused and accurate protein generation, effectively closing the loop between design and evaluation.

We demonstrated the capability of this platform by designing a cell-penetrating peptide (CPP) that binds readily to the CXCR4 cell-surface receptor while exhibiting minimal binding to the NRP1 receptor. We first trained a generative AI model on a diverse set of known CPP sequences to produce one million candidate sequences. These candidates were then subjected to molecular docking and molecular dynamics (MD) simulations, allowing us to estimate binding free energies for both CXCR4 and NRP1 *in silico*. A multi-objective Bayesian optimization was performed to maximize CXCR4 affinity while concurrently minimizing NRP1 affinity, thereby guiding the design toward peptides with strong on-target binding and weak off-target interactions. Through this process, we identified a promising CPP candidate predicted to achieve selective delivery to CXCR4-expressing cells. This candidate is currently being evaluated in cell-based experiments to confirm its selective uptake by target cells.

In conclusion, this study demonstrates the potential for highly efficient and precise protein and peptide design through the integration of AI, computational simulations, and experimental validation in a closed-loop approach. Using selective drug delivery to receptor-specific cells as an example, our results highlight how a deliberate, feedback-driven design strategy can move protein design away from reliance on serendipity and toward a more deterministic, targeted design process.

Keyword

Protein Design, DBTL Cycle, Generative AI, MD Simulation, Bayesian Optimization



Short biography

Ph.D. in Information Science and Technology at The University of Tokyo (2019); Research Associate at The University of Tokyo (2019–2021); Designated Associate Professor at Nagoya University (2021–2022); Project Associate Professor, then Associate Professor at Tokyo Medical and Dental University and Institute of Science Tokyo (2023–); Project Scientist at Innovation Center of NanoMedicine (2025–).

Specialty and present interests: I specialize in computational protein engineering and design. Currently, I am particularly interested in autonomous, closed-loop protein design frameworks that integrate AI-driven generation, computational simulation, and robotic experimentation—a “lab-in-the-loop” paradigm that seamlessly bridges *in silico* modeling with *in vitro* validation.

References

Hayashi S, Hayashi Y, Koseki J, Shimamura T. De novo design of BCAT1 inhibitory proteins via a self-improving AI-MD integrated cycle. The 33rd Annual Intelligent Systems for Molecular Biology and the 24th Annual European Conference on Computational Biology. 2025.

Yamahata I, Hayashi S, Koseki J, Shimamura T. Deep learning-based design of receptor selective cell-penetrating peptides. The 1st Asia & Pacific Bioinformatics Joint Conference. 2024.

Hayashi S, Koseki J, Shimamura T. In silico DBTL cycle platform to design highly functional de novo proteins. The 23rd European Conference on Computational Biology. 2024.

Session 2　17:00-17:25

Automating Molecular Discovery with an Integrated Platform of AI, Robotics, and 3D-Phenomics

Dr. Hideyuki SHIMIZU

M&D Data Science Center, Institute of Integrated Research, Institute of Science Tokyo

Abstract

The escalating threat of antimicrobial resistance (AMR), projected to become a leading cause of death by 2050, demands new therapeutic classes. Antimicrobial peptides (AMPs) offer a promising solution, as they are less likely to induce resistance. Our laboratory has developed AMP-Atlas, an advanced AI platform that predicts both the presence (AMP-likeness) and potency of antimicrobial activity from amino acid sequences alone, utilizing large protein language models and contrastive learning.

We deployed this AI using three complementary strategies. First, by mining natural diversity, we screened 729,445 uncharacterized peptides from UniProt. Our AI identified a novel peptide from *Drosophila*, which experimental validation confirmed possesses potent activity comparable to ampicillin. Second, by uncovering cryptic peptides, we performed *in silico* digestion of the human proteome. We synthesized 20 AI-predicted candidates and found that 18 (90%) exhibited potent antimicrobial activity, with many exceeding the efficacy of conventional antibiotics. Third, we implemented an *in silico* evolutionary strategy to design novel AMPs. This approach generated 10 new peptides, 7 of which showed significantly stronger activity than both ampicillin and their parent sequences. In total, our AI-driven platform has enabled the discovery and *de novo* design of 29 novel, active AMPs.

Beyond antimicrobial discovery, our laboratory is addressing the high costs and lengthy timelines of traditional drug R&D by developing CellCloud, an integrated platform for next-generation drug screening that combines robotic automation with AI-driven analysis. The fundamental limitation of conventional screening is its reliance on simplistic 2D cell cultures, which often fail to predict human responses. CellCloud overcomes this by automating the entire pipeline for 3D patient-derived organoid screening. By integrating robotic liquid handling for compound perturbation, automated high-throughput 3D imaging, and deep learning for complex 3D phenotypic analysis, our platform establishes a new paradigm for AI-driven drug discovery. This approach enables us to screen massive compound libraries against more physiologically relevant models, accelerating the identification of novel therapeutics for intractable diseases.

Keyword

AI-driven drug screening, 3D organoid phenomics, Computational peptide design, Automated therapeutic development

Short biography

Hideyuki SHIMIZU received his M.D. from Tohoku University School of Medicine in 2012. After completing his clinical residency, he engaged in basic medicine and life science research at Kyushu University, where he earned a Ph.D. in Medical Science. Following his research at institutions such as the Department of Systems Biology at Harvard Medical School and the Synthetic Biology Center at MIT, he has joined at Tokyo Medical and Dental University (now Institute of Science Tokyo) in 2022.

He has consistently been involved in research dedicated to creating the future of medicine. Currently, he is conducting over 50 collaborative projects across industry, academia, and government, focusing on areas including cancer, molecular biology, bioinformatics, medical AI systems, drug discovery, quantum computing, and synthetic biology.

Specialty and present interests

Systems Biology, Drug Discovery, Bioinformatics

References

Otani Y., Koga D., Wakizaka Y., Shimizu H. AMP-Atlas: Comprehensive Atlas of Antimicrobial Peptides to Combat Multidrug-resistant Bacteria, ***bioRxiv***, 2025.

Sakuma T., Otani Y., Shimizu H. High-Resolution Mapping of the Human E3-Substrate Interactome using Ubicon Uncovers Network Architecture and Cancer Vulnerabilities, ***bioRxiv***, 2025.

Shimizu H., Kodama M., Matsumoto M., Orba Y., Sasaki Y., Sato A., Sawa H., Nakayama KI. LIGHTHOUSE illuminates therapeutics for a variety of diseases including COVID-19, ***iScience***, 2022.