口頭発表リスト Oral Presentation List

発表番号 No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation
O01（Drug Discovery Application(1)） October 29 (Tue) 14:00-15:30 401 Meeting room(4F)			
O01-01	Ella Morishita	Veritas In Silico Inc.	Unveiling the Potential of RNA-Targeted Small Molecule Therapies: Innovations in Computational and Biophysical Approaches
O01-02	Atsushi Matsuo	Chugai Pharmaceutical Co.,Ltd	Computational Chemistry and Structure-Based Molecular Design for a Cyclic Peptide Drug Discovery Platform
O01-03	Syunya Suzuki	Nagoya University	Machine learning approach to analyze DNA-encoded library screening data for hit identification
O01-04	Yuki Matsukiyo	Kyushu Institute of Technology	Scaffold-retained molecule generation considering gene expression profiles with deep learning
O01-05	Takamasa Suzuki	Tokyo Institute of Technology	Development of a Molecular Generative model via the Decoupled Setting on Multi-objective Bayesian Optimization
O01-06	Donny Ramadhan	Osaka University	Optimizing Multitask Learning with Evolutionary Metrics for Enhanced QSAR-based Natural Product Activity Prediction
O02（Data Science(1)） October 30 (Wed) 10:00-11:30 Training room(4F)			
O02-01	Tomoyasu Sugiyama	Tokyo University of Techmology	Deep leaning of new morphological characteristics of blood vessel in breast cancer.
O02-02	Rintaro Yashiro	Tokyo Institute of technology	Enhancing Drug-Target Interaction Prediction using Large Language Models and Low-Rank Adaptation
O02-03	Shuya Nakata	Kobe University	Exploring Synthetically Accessible Chemical Spaces with Product-of-Expert Chemical Language Models
O02-04	Kotaro Kamiya	SyntheticGestalt KK	Feature Design of Molecular 3D Structures for Fast Approximate Nearest Neighbor Search
O02-05	Shumpei Nemoto	The University of Tokyo	Clmpy: A platform for Chemical Language Model comparable training and structure generation ability
O02-06	Pavel Sidorov	Institute for Chemical Reaction Design and Discovery (ICReDD)	Fragment descriptors in predictive modeling for molecules and reactions
O03（Drug Discovery Application(2)） October 30 (Wed) 10:00-11:30 401 Meeting room(4F)			
O03-01	Piyatida Natsrita	Osaka University	Construction of Flavivirus database and therapeutic antibody discovery using machine learning algorithm
O03-02	Mori Kenichi	Astellas Pharma Inc.	Digital Transformation on Small Molecule Optimization Research at Astellas Pharma
O03-03	David Jimenez Barrero	Elix, Inc	Open Molecule Generator: A Multipurpose Molecule LLM
O03-04	Yosui Nojima	Osaka University	Application of machine learning to single-cell RNA sequencing provides the candidate drugs against drug-tolerant persister cells in colorectal cancer
O03-05	Hayato Tsumura	Department of Biomedical Data Intelligence, Graduate School of Medicine, Kyoto University	Predicting Novel Therapeutic Target Molecules Using Neural Networks: Validation and Applicability to Unknown Diseases
O03-06	Iori Yamahata	Nagoya University Graduate School of Medicine	Design of Receptor Selective Cell-Penetrating Peptides Using Deep Learning and Simulations

O04 (Molecular Robotics(1)) **October 30 (Wed) 10:00-11:30** **407 Meeting room(4F)**			
O04-01	Tsuyoshi Inaba	Grad.Sci.Eng.,Tohoku Univ	Biomimetic Multicellular Lipid-Based Membranes for Stimulus-Responsive Drug Delivery
O04-02	YIMING GONG	Kyoto University	Physical Reservoir Computing Device Using Active Matter Composed of a Swarm of Biomolecular Motors.
O04-03	Soichiro Hiroi	Graduate School of Arts and Science, The University of Tokyo	GAN-Based Multi-Axis Resolution-Enhanced 3D Visualization of Giant Vesicles
O04-04	Haruto Obuchi	The University of Tokyo, Graduate School of Arts and Sciences, Department of Basic Science	Investigation on heterogeneous pairs of cell-sized liposomes formed in a microfluidic device
O04-05	Ibuki Kawamata	Kyoto University	Integrated web user interface for DNA nanotechnology including coarse-grained molecular dynamics simulation
O04-06	Hirotaka Kondo	Kansai University	Development of a Supervised Deep Learning Method for DNA Sequence Estimation from DNA Images
O05 (Quantum-Structural Life Sscience, ADME/toxicity, Bioinformatics) **October 30 (Wed) 10:00-11:30** **406 Meeting room(4F)**			
O05-01	Yuga Moriyama	Yamanishi Laboratory, Department of Complex Systems Science, Graduate School of Informatics, Nagoya University	AlphaFold protein 3D structures enhance genome-wide scale compound-protein interaction prediction with deep learning
O05-02	Kazuyoshi Yoshii	ZERIA Pharmaceutical Ltd., Co.	The effect of food on pharmacokinetics of acotiamide for the treatment of functional dyspepsia
O05-03	Flora R. Aigbe	Osaka University	Computational exploration of bipolar disorder multi-omics data in the quest for novel drug targets
O05-04	Nina Holsmoelle	Osaka University	Learning the Language of Life: Feasibility of Using LLMs to Understand Latent Characteristics of Proteins from Residue Structural Environments
O05-05	Tatsunori Osone	Okayama University	SGCRNA: A Novel Tool for Gene Co-Expression Network Analysis Using Spectral Clustering
O05-06	Reiko Watanabe	Institute for Protein Research, Osaka University	Exploring cancer treatment candidates targeting chromatin remodeling factors
O06 (Data Science(2), Clinical Application) **October 31 (Thu) 10:00-11:30** **Training room(4F)**			
O06-01	Tsuyoshi Kimura	Nagoya University	3D structure-based chemical foundation model to predict the bioactivity and toxicity
O06-02	Yuto Matsumoto	Yokohama National University	Comparison Between Word Embeddings and Molecular Descriptors by Clustering and Distribution Analysis from Antioxidant Articles
O06-03	Yasuhiro Yoshikai	The University of Tokyo Graduate School of Pharmaceutical	Reconstructable latent representation of molecules by Graph Transformer VAE
O06-04	Tomoki Kawano	Graduate School of Agricultural and Life Sciences, The University of Tokyo	Towards the Design of Natural Product Biosynthetic Gene Clusters Using Natural Language Processing Technology
O06-05	MASAKAZU SEKIJIMA	Tokyo Institute of Technology	Design of Novel Compounds Through Protein-Ligand Interaction-Based Generative Methods
O06-06	Yuji Sakahashi	National Cerebral and Cardiovascular Center	Analysis of the usefulness of AlphaMissense score for predicting protein function. -Evaluation by *GLA*, the causative gene of Fabry disease-

O07 (Drug Discovery Application(3)) **October 31 (Thu) 10:00-11:30** **401 Meeting room(4F)**			
O07-01	Joshua Owoyemi	Elix, Inc.	SynthFormer: A Customizable Framework for Virtual Synthesis-Based Molecule Generation
O07-02	Takashi Matsumoto	Rigaku Corporation	Relationship between cyclic peptide structure in solution and membrane permeability
O07-03	Hideto Hoshino	Nagoya University	Efficient docking simulation-based generation of bioactive compounds with deep generative models
O07-04	Casey J. Galvin	Elix, Inc.	Optimization of Generator Reward Function Settings for Non-covalent KRAS Inhibitors
O07-05	Kazuma Kaitoh	Nagoya University	Development of Scaffold and Fragment Definition Algorithms with a Case Study on Chemical Library Analysis
O07-06	Yukinobu Matsuno	Tokyo Tech	Deep Learning-Based Protein-Protein Interaction Prediction Considering Angle Information
O08 (Computational Chemistry (Molecular Modeling)(1)) **October 31 (Thu) 10:00-11:30** **407 Meeting room(4F)**			
O08-01	Takeshi Ishikawa	Kagoshima University	Quantum Chemistry-Based Protein-Protein Docking without Any Empirical Parameters
O08-02	Mochammad Arfin Fardi	Osaka University	Prediction and Analysis of Protein-Ligand Complexes Through R-value Analysis of High-Temperature Molecular Dynamics Simulation
O08-03	Atsuhiro Tomita	Preferred Networks, inc.	Conditional structure prediction of protein-compound complex
O08-04	Ai Shinobu	Osaka University	Integrating Mathematical Modeling and Molecular Dynamics Simulations to study the effect of EGFR Mutations in Lung Cancer
O08-05	Natsuki Kanazawa	Graduate School of Medicine, Kyoto University	Large-Scale MD-Based CPI Prediction Using Supercomputer Fugaku
O08-06	Chiduru Watanabe	RIKEN BDR	Progress of data collection in FMO database and efforts to evaluate structural qualities of biological macromolecules using quantum chemical interaction energy analysis
O09 (Molecular Robotics(2), Data Science(3) Computational Chemistry (Molecular Modeling)(2)) **October 31 (Thu) 10:00-11:30** **406 Meeting room(4F)**			
O09-01	Shin-ichiro M. Nomura	Graduate school of Engineering, Tohoku University	Towards the Construction of Next-Generation Molecular Robots with Quick Motion and Information Processing
O09-02	Ken Komiya	Japan Agency for Marine-Earth Science & Technology (JAMSTEC)	Experimental validation of a modified Whiplash PCR for profiling temporal and coexistence patterns of nucleic acids
O09-03	Kazuyoshi Ikeda	RIKEN	Development of a sustainable database for middle molecules using AI-driven data curation
O09-04	Shuichiro Makigaki	Kitasato Institute	Designing an Information Infrastructure for the Integration and Utilization of Multimodal Bioactivity Information
O09-05	Gergely Juhasz	Tokyo Institue of Technology	Leveraging LLMs for Quantum Chemistry: A Comparative Study of Input File Generation for Gaussian, DFTB+, and ORCA
O09-06	Suyong Re	National Institutes of Biomedical Innovation, Health and Nutrition (NIBIOHN)	Structure and stability of glycan interaction network on the HIV envelope glycoprotein