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 臨床インフォマティクス Clinical Informatics			
O01-01	Yuto Takemoto	Department of Integrated Health Sciences, Graduate School of Medicine, Nagoya University	Robustness comparison of data preprocessing methods for exosome-derived miRNA microarray data
O01-02	Iori Azuma	Laboratory of Molecular Pharmacokinetics, Graduate School of Pharmaceutical Sciences, The University of Tokyo	GLDADec: Guided LDA deconvolution enabled us to identify cell type proportions
O01-03	Kazuki Fujiwara	Ajinomoto Co., Inc.	Development of the classification model for groups with relatively lower hippocampal volume using blood amino acid levels
O01-05	Takafumi Ojima	Osaka University	Body mass index stratification improves polygenic prediction of type 2 diabetes in trans-biobank analysis
O01-06	Hiroko Terui-Kohbata	Tokyo Medical and Dental University	An innovative attempt to assist REC procedure for the medical research involving samples and information held by national network
O02 分子ロボティクス/バイオインフォマティクス Molecular Robotics/Bioinformatics			
O02-01	Hirotaka Kondo	Kansai University	Development of a Prototype of voice-operated VR Molecular Design Environment
O02-02	Soichiro Hiori	Graduate School of Arts and Science, The University of Tokyo	Deep Learning-Based Deconvolution of Confocal Laser-scanning Fluorescence Microscopy Images for Enhanced Visualization of Giant Vesicles
O02-03	Yuhui Zhang	Tokyo Institute of Technology	Large-scale VR Molecular Rendering for Co-creation Environment
O02-04	Narumi Hatano	Graduate School of Medicine and Faculty of Medicine Kyoto University	Application of Machine Learning Models in Prediction of Disease Therapeutic Target Molecules Using Gene Expression Profiles
O02-05	Yuki Kuniyoshi	Otsuka Pharmaceutical Co., Ltd.	Gene prioritization using a genetics-led approach for target discovery of ALS
O02-06	Satoshi Nagaie	Tohoku University Tohoku Medical Megabank Organization	Elucidation of trajectories from healthy state to mibyo and disease onset through large-scale specific health checkup data
O03 ケムインフォマティクス・機械学習/AIによる創薬研究 Cheminformatics, machine learning, AI-based drug discovery			
O03-01	Yuki Matsukiyo	Kyushu Institute of Technology	De novo inhibitor and activator design from gene expression profiles via deep learning and Bayesian optimization
O03-02	Yasuhiko Nakao	Nagasaki University Hospital	Development of 53BP1 expression classification model by using Segment-Anything Model(SAM) and CNN Model in pathological image
O03-03	Tatsuya Yoshizawa	Yokohama City University	Multi-objective Molecular Structure Generation Using Dynamic Applicability Domains Adaptation
O03-04	Shinnosuke Takada	Kyushu Institute of Technology	Generating Synthesizable Compound Structures with Desired Properties via Deep Learning Models
O03-05	Vincent Paul Guillaume Richard	Elix, Inc.	Benchmarking Deployed Generative Models on Elix Discovery
O03-06	Haris Hasic	Tokyo Institute of Technology	Improving the Practical Applicability of Computer-assisted Chemical Synthesis Planning Approaches using Substructure Patterns
O03-07	Chiduru Watanabe	RIKEN BDR	Development of Auto-FMO protocol and data accumulation in FMODB through 2023
O04 計算化学（分子計算）/創薬応用/量子構造生命科学 Computational Chemistry (Molecular Modeling) / Drug Discovery Application/Quantum-Structural Life Science/Computer-Aided Drug Design			
O04-01	Mochammad Arfin Fardiansyah Nasution	Osaka University	Exploring the Selectivity and Binding Mechanism of ToP-DNJ Toward Endoplasmic Reticulum α-Glucosidase II
O04-02	Suyong Re	National Institutes of Biomedical Innovation, Health and Nutrition	In-silico design of peptide inhibitors containing unnatural amino acid
O04-03	Haruka Kono	Tokyo Institute of Technology	Analysis of the binding profile of *quinonoid*-form of dihydropteridine to *quinonoid*-dihydropteridine reductase
O04-04	Risa Shiozawa	Tokyo Institute of Technology	Study Improves Performance of Pocket Comparisons Using Machine Learning
O04-05	Yuto Komeiji	AIST	Fundamentals of Molecular Dynamics Simulation
O04-06	Takashi Matsumoto	Rigaku Corporation	MAXS reveals a disorder-to-order transition of the intrinsically disordered region in active MAP2K6
O04-07	Jack Yan	Wuxi Biortus Biosciences Co. Ltd.	Near atomic-resolution cryoEM structure of PROTAC ternary complex
O05 計算化学（分子計算）/創薬応用/量子構造生命科学 Computational Chemistry (Molecular Modeling) / Drug Discovery Application/Quantum-Structural Life Science/Computer-Aided Drug Design			
O05-01	Ai Shinobu	Osaka University	Molecular details on the binding of inhibitors to c-Src kinase revealed by molecular dynamics simulations
O05-02	Shun Yokoi	Meiji University	Structural and Computational Insight into Dynamics and Intermediate State in Activation of Orexin 2 Receptor
O05-03	Ryunosuke Yoshino	University of Tsukuba	Conformation Search of Ternary Complexes for Rational PROTAC Linker Design Using Enhanced Sampling Method
O05-04	Jumpei Morimoto	The University of Tokyo	Conformational studies of oligo(*N*-methylalanine) and application of the oligomer for designing a ligand against a cancer-related protein MDM2
O05-05	Osamu Ichihara	Schrödinger KK	Uncovering the Mechanism of Molecular Glue Protein Degraders：The high energy water molecules at the P-P interface play key roles in the recruitment of RBM39 to DCAF15
O05-06	Takamasa Suzuki	Tokyo Institute of Technology	Development of hit-to-lead molecular optimization by multi-objective Monte Carlo Tree Search

O06 分子認識と分子計算/創薬応用 Moleuclar recognition and Molecular modeling/Drug Discovery Application			
O06-01	Song-Ho Chong	Kumamoto University	Changes in the conformational landscape of Src kinase upon substrate recognition
O06-02	Ryosuke Kita	Kyushu University	Development of a machine learning model for predicting protein-ligand interactions based on FMO data
O06-03	Hiromu Matsumoto	Kyushu University	Utilizing the FMO Database for Transfer Learning in Constructing Machine Learning Force Fields for Biomolecular Systems.
O06-04	Yuma Handa	Hoshi University	Understanding the RNA Sequence Specificity of Translation Initiation Factor Inhibitors through Dynamical FMO Analysis
O06-05	Hiromitsu Shimoyama	Noguchi Institute	Free Energy Analysis of FtsXECL1 Domain Motion by Divide-and-Conquer MD simulation
O06-06	Kasumi Yasuda	Dept. of Bioscience and Bioinformatics, Faculty of Comp Sci and Systems Eng, Kyushu Institute of Technology	Transformer Encoder-based Generative Adversarial Network for Design of Polypharmacological Drugs
O07 データサイエンス/ADME・毒性 Data science/ADMET			
O07-01	Kazuyoshi Yoshii	Zeria Pharmaceutical Co., Ltd.	In silico and in vitro studies for identification of UDP-glucuronosyltransferase isoforms in acotiamide metabolism
O07-02	Chen Li	Nagoya University	Scaffold-Retained Transformer GAN for Molecular Generation with Chemical Property Optimization
O07-03	Shinya Ishihara	Kyushu Institute of Technology	Computational prediction of target molecules of drug candidate compounds from cell morphology images
O07-04	Takuto Koyama	Kyoto University	Insight into Federated Learning for Compound-Protein Interaction Prediction
O07-05	Thomas Auzard	Elix, Inc.	Binding Compound Database Screening using Deep Learning: Strategies for Improved Candidate Enrichment
O07-06	Nathan Robert Lugg	SyntheticGestalt	AdaSplit: an adaptive dataset split method
O08 分子ロボティクス Molecular Robotics			
O08-01	Ken Komiya	Japan Agency for Marine-Earth Science & Technology	Experimental Investigation of Cascaded DNA Generation Reaction as A Signal Amplification Circuit
O08-02	Aoi Takeguchi	Ochanomizu University	Efficient DNA-based structure automated exploration with machine-learning models
O08-03	Shin-ichiro M. Nomura	Graduate school of Engineering, Tohoku University	Lipid Based Artificial Multicellular Systems for Compartmentalized and Stimuli-Responsive Drug Delivery
O08-04	Chen Ma	Tokyo Institute of Technology	3D Point Cloud Analysis of Microtubule Motility Dynamics
O08-05	Xiaoran Hu	Tokyo Institute of Technology	High-Resolution AFM Imaging of DNA Structures: An Approach via Cycle GANs and Virtual Reality Integration
O08-06	Keita Abe	Tohoku University	DNA reaction–diffusion model with polymerization for pattern formation