発表番号 No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation	発表日 Poster Day	発表時間 Poster Time
分子認識と分子計算 Moleuclar recognition and Molecular modeling					
P01-01☆	Kairi Furui	Tokyo Institute of Technology	Design of scalable perturbation maps for relative free energy calculations	October 24 (Tue)	15:30-16:15
P01-02☆	Marin Yokomine	Graduate School of Engineering, The University of Tokyo	In silico screening of protein-protein interaction inhibitors using oligo(*N*-methylalanine) as a scaffold	October 24 (Tue)	16:15-17:00
P01-03☆	Mariko Ibara	Kindai University	Interaction analysis of Keap1 and the inhibitors using Fragment Molecular Orbital Method.	October 25 (Wed)	15:30-16:15
P01-04	Shun Sakuraba	National Institutes for Quantum Science	FEP-suite: free-energy calculation pipelines for biomolecules	October 25 (Wed)	16:15-17:00
P01-05☆	Sota Tanaka	School of Pharmaceutical Sciences, Osaka University	Construction of a system for predicting the activity of low-molecular-weight compounds using FMO calculations	October 24 (Tue)	15:30-16:15
P01-06☆	Tomoya Nabetani	Yokohama city university	Evaluation of MD-based high-throughput screening methods using supercomputer Fugaku	October 24 (Tue)	16:15-17:00
P01-07☆	Yukina Nakai	Graduate School of Medical Life Science, Yokohama City University	Binding Pathway of Hydroxycarboxylic acid receptor 2 (HCAR2) — Niacin Explored by Tree-Search Molecular Dynamics (TS-MD)	October 25 (Wed)	15:30-16:15
P01-08☆	Shinji Iida	Kitasato University	Exploring Cryptic Binding Sites through Noble Gas Interactions	October 25 (Wed)	16:15-17:00
P01-09	Hirofumi Watanabe	WithMetis Co., Ltd.	Practical visualization of interaction energies by FMO for drug design II: Updates and improvements	October 24 (Tue)	15:30-16:15
P01-10☆	Hiroto Asano	Osaka University	Applicabilities of Neural Network Potential to Predict ligand-RNA Interactions	October 24 (Tue)	16:15-17:00
P01-11☆	Kenta Kamimura	Hoshi University	Computational Interaction analysis between Interleukin10 and Interleukin10 receptor Using the Fragment Molecular Orbital Method	October 25 (Wed)	15:30-16:15
P01-12☆	Toma Miyagishi	School of Pharmaceutical Sciences, Osaka University	Interaction analysis of IL-10 receptor complex using MD and FMO calculations	October 25 (Wed)	16:15-17:00
P01-13☆	Ozora Kudo	Nihon University	Conformational behavior, dynamics, and affinity of A18-modified aptamers toward human Immunoglobulin G	October 24 (Tue)	15:30-16:15
P01-14☆	Shu Ono	School of Pharmaceutical Sciences, Osaka University	Structure and interaction analysis of complexes between BzDANP and bulged RNAs using NMR and dynamical FMO calculation	October 24 (Tue)	16:15-17:00
P01-15☆	Kowit Hengphasatporn	筑波大学	Finding Potent HIV-1 Protease Inhibitors through FMO-Guided Drug Design	October 25 (Wed)	15:30-16:15
計算化学（分子計算） / 創薬応用 Computational Chemistry (Molecular Modeling) / Drug Discovery Application					
P02-01☆	Kentaro Takai	Fujitsu Ltd.	Comparing predicted structures of cyclic peptides in solvent to experimentally measured structures in complex	October 25 (Wed)	16:15-17:00
P02-02☆	Seigo Yumura	Osaka Metropolitan University	Conserved gatekeeper methionine determines accessibility to the ATP-sites and selectivity among MAP2K1/4/7	October 24 (Tue)	15:30-16:15
P02-03☆	Yuki Shimizu	Kyoto University	Protein Dynamics Prediction using Video Prediction AI: An Alternative to Traditional MD Simulations	October 24 (Tue)	16:15-17:00
P02-04☆	Mark McGann	OpenEye, Cadence Molecular Sciences	FastROCS Plus in Orion®: Not Just Ligand-Based Virtual Screening in Billion Scale	October 25 (Wed)	15:30-16:15
P02-05☆	Ryuichiro Hara	Cresset	Validation of Docking against an Ensemble of Molecular Dynamics Snapshots	October 25 (Wed)	16:15-17:00
P02-06☆	Chie Motono	National Institute of Advanced Industrial Science and Technology (AIST)	A search method for novel protein functional site based on the spatial distribution of disease-associated missense variants	October 24 (Tue)	15:30-16:15
P02-07☆	Hajime Sugiyama	Mitsubishi Chemical Corporation	Insight into the Binding Modes of Allosteric ERK2 Inhibitors using Metadynamics Simulations	October 24 (Tue)	16:15-17:00
P02-08☆	Junya Yamagishi	Preferred Networks	Evaluation of Neural Network Potentials on Drug-like Molecules and Applications in Drug Discovery	October 25 (Wed)	15:30-16:15
P02-09	Mizuki Takemoto	Preferred Networks Inc.	Development of free energy calculation pipeline in Preferred Networks	October 25 (Wed)	16:15-17:00
P02-10☆	Keisuke Yanagisawa	Tokyo Institute of Technology	Quantitative Estimation of Protein-Chemical Substructure Interaction with Inverse Mixed-Solvent Molecular Dynamics Simulation	October 24 (Tue)	15:30-16:15
P02-11☆	Genki Kudo	University of Tsukuba	Comprehensive structual analysis of PROTAC mediated ternary complexes using enhanced conformational sampling methods	October 24 (Tue)	16:15-17:00
P02-12☆	Uika Koshimizu	Dept. of Chemistry & Biochemistry, School of Advanced Science and Engineering, Waseda Univ	Discovery and evaluation of potent covalent inhibitors targeting SARS-CoV-2 main protease by hybrid *in silico* drug study	October 25 (Wed)	15:30-16:15

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					
P03-01☆	Mariko Yokogawa	Keio University	Discovery of the middle-sized compounds inhibiting the SARS-CoV-2 viral entry, using *in silico* approach and NMR analysis	October 25 (Wed)	16:15-17:00
P03-02☆	Toshiaki Watanabe	DAIICHI SANKYO CO., LTD.	Development of Chemical Similarity Search Tool for Hit-Expansion Research.	October 24 (Tue)	15:30-16:15
P03-03☆	Wenxing Hu	Tokyo Institute of Technology	Spatial Predictions of Protein-Protein Interaction with AlphaFold Multimer	October 24 (Tue)	16:15-17:00
P03-04	Chisato Kanai	INTAGE Healthcare Inc.	Optimization of DDR1 inhibitor with a desired Pharmacophore using Deep Reinforcement Learning	October 25 (Wed)	15:30-16:15
P03-05☆	Yusuke Tateishi	Graduate School of Science and Technology, Kumamoto University	Natural Product Drug Discovery by Electronic-Structure Informatics: Search for Novel α-glucosidase Inhibitors	October 25 (Wed)	16:15-17:00
P03-06☆	Yusuke Tsutsumi	Kumamoto University	Computational-Model-Based Machine-Learning Prediction of Regioselectivity in Organic Reactions: Application to Electrophilic Attach to Quinone Derivatives	October 24 (Tue)	15:30-16:15
P03-07☆	Jun Nakabayashi	Analysis Technology Center, FUJIFILM Corporation	AI-AAM. Increasing the number of active compounds with various scaffolds and substituents from one active compound	October 24 (Tue)	16:15-17:00
P03-08☆	Ryuto Koyagi	Tokyo Institute of Technology	Prediction of gut microbiota from questionnaire data using machine learning	October 25 (Wed)	15:30-16:15
P03-09☆	Hiroaki Iwata	Kyoto University	A New Molecular Generation Model Combining Deep Learning and Reinforcement Learning	October 25 (Wed)	16:15-17:00
P03-10☆	Taisei Kakibuchi	Fujitsu Ltd.	Explainable AI Analysis for Accelerating Drug Discovery of Sequence Modalities.	October 24 (Tue)	15:30-16:15
P03-11☆	Yasuhiro Yoshikai	Graduate School of Pharmaceutical Sciences, The University of Tokyo	Investigation on the Transformer’s learning process of chemical structure comprehension	October 24 (Tue)	16:15-17:00
P03-12	Kikuko Kamisaka	RIKEN Center for Biosystems Dynamics Research	Recent developments of FMODB: Enhancement of search functionality	October 25 (Wed)	15:30-16:15
P03-13☆	Shuya Nakata	Kobe University	Composing Property-Specific SMILES Language Models for Multi-Objective Drug-Like Molecule Generation	October 25 (Wed)	16:15-17:00
P03-14☆	Apakorn Kengkanna	Tokyo Institute of Technology	Enhancing Model Learning and Interpretation Using Multiple Molecular Graph Representations for Compound Property and Activity Prediction	October 24 (Tue)	15:30-16:15
データサイエンス Data science					
P04-01☆	Chihiro Higuchi	National Institutes of Biomedical Innovation, Health and Nutrition (NIBIOHN)	Japanese food ontology and knowledge graph as its application	October 24 (Tue)	16:15-17:00
P04-02☆	Kosuke Takeuchi	DAIICHI SANKYO CO., LTD.	Development of efficient process to extract SAR knowledge from literature by using CCR algorithm	October 25 (Wed)	15:30-16:15
P04-03☆	Atsushi Midorikawa	WorldFusion Co,. Ltd.	Classification and Comparison of Gene-Disease Associations using BioBERT and PubMedBERT on GeneRIF Data	October 25 (Wed)	16:15-17:00
P04-04	Shuya Ikeda	Database Center for Life Science	TogoID: ID conversion service as a basis for life science database integration	October 24 (Tue)	15:30-16:15
P04-05☆	MARTIN -	Osaka University	Prediction of Xanthine Oxidase Inhibitors using Graph Neural Network	October 24 (Tue)	16:15-17:00
P04-06☆	Yuki Moriya	ROIS-DS	TogoDX/Human: An application for integrated exploration of human-related data	October 25 (Wed)	15:30-16:15
P04-07☆	Shumpei Nemoto	The University of Tokyo	Elucidation of CLM-based deep generative model with high translation accuracy as a generator of virtual chemical libraries with diverse structures	October 25 (Wed)	16:15-17:00
P04-08☆	Shuichi Kawashima	Research Organization of Information and Systems	Advancements in the RDF portal: Enriching cheminformatics insights	October 24 (Tue)	15:30-16:15
P04-09☆	Thanawat Tangpornpisit	Kanazawa University	3D packing for enhancing extended depth of field microscopy images	October 24 (Tue)	16:15-17:00
分子ロボティクス Molecular Robotics					
P05-01☆	Yuki Minamide	Kansai University	Long-range energy transfer using DNA-scaffolded BRET system	October 25 (Wed)	15:30-16:15
P05-02☆	Shogo Kai	Sch. Comp. Sci. Syst. Eng., Kyutech	Regulation of spatiotemporal formation of DNA droplets	October 25 (Wed)	16:15-17:00
P05-03☆	Hiroaki Ohno	Sch. Comp. Sci. Syst. Eng., Kyutech	Phase-separated microstructures with sequence-designed DNA and peptides	October 24 (Tue)	15:30-16:15
創薬応用 Drug Discovery Application					
P06-01	Masataka Kuroda	National Institutes of Biomedical Innovation, Health and Nutrition	Miné Tools Common: Open Platform to Accelerate Drug Discovery	October 24 (Tue)	16:15-17:00
P06-02	Mao Tanabe	National Institutes of Biomedical Innovation, Health and Nutrition	Application of AI-AAM, an *in silico* scaffold hopping method, to the drugs for rare and intractable diseases	October 25 (Wed)	15:30-16:15

P06-03	Kentaro Kawai	Setsunan University	Development of a model for predicting binding poses of ROR γ inhibitors using machine learning with ligand coordinate profile.	October 25 (Wed)	16:15-17:00
P06-04☆	Yusuke Tateno	SHIONOGI & CO., LTD.	Development of a web based de novo design tool for medicinal chemists	October 24 (Tue)	15:30-16:15
P06-05	Atsushi Yoshimori	Institute for Theoretical Medicine, Inc.	Web-based system for detecting SAR transfer events from SAR progression data of different targets	October 24 (Tue)	16:15-17:00
P06-06☆	Keisuke Uchikawa	Tokyo Institute of Technology	Identifying suitable AlphaFold2 protein structure models for improved structure-based virtual screening	October 25 (Wed)	15:30-16:15
P06-07☆	Hiroki Anzai	The University of Tokyo	The construction of vNAR library by cDNA display system for application to drug discovery	October 25 (Wed)	16:15-17:00
P06-08☆	Kazuma Kaitoh	Nagoya University	Chemical Space Analysis for Cytochrome P450–Induced Orphan Nuclear Receptors Ligands	October 24 (Tue)	15:30-16:15
P06-09☆	Ryosuke Nagasawa	Tohoku Univ.	Development of novel fluorescent indicators to discover new RNA-targeting small molecules in FID assay driven by large-scale profiles of RNA-indicator interactions	October 24 (Tue)	16:15-17:00
P06-10☆	Koujin Kojima	Keio University Graduate School of Pharmaceutical Sciences	Structural basis of the inhibition of the Keap1-Nrf2 interaction by novel PPI inhibitors discovered by machine learning	October 25 (Wed)	15:30-16:15
ADME・毒性 ADMET					
P07-01☆	Kaoru Takadera	Institute for Protein Research, Osaka University	In silico regression modelling to predict the transport inhibitory activity of Breast Cancer Resistant Protein	October 25 (Wed)	16:15-17:00
P07-02☆	Kan Shiraishi	Daiichi Sankyo Co., Ltd.	Automation of building ML prediction models using in-house data and development of prediction result response applications	October 24 (Tue)	15:30-16:15
P07-03☆	Yuki Umemori	TEIJIN PHARMA LIMITED	Novel in silico model to predict the risk of covalent binding and investigation of important substructures using by Message Passing Neural Network	October 24 (Tue)	16:15-17:00
P07-04☆	Koji Jojima	Chemicals Evaluation and Research Institute, Japan	Development of the classification model to predict the potential of chemical reactivity to cysteine using the combination of two machine learning algorithms	October 25 (Wed)	15:30-16:15
P07-05	Yuto Itami	National Institute for Environmental Studies	Performance Evaluation for Algal Acute and Chronic Toxicity Prediction of QSAR Model “KATE2020 ver. 4.1”	October 25 (Wed)	16:15-17:00
P07-06☆	Hitoshi Kawashima	National Institutes of Biomedical Innovation, Health and Nutrition	An Attempt to Modify Training Datasets Containing Inequality Signs for Machine Learning	October 24 (Tue)	15:30-16:15
P07-07☆	Fukino Kono	Faculty of Pharmacy, Kanazawa University	Physiologically based pharmacokinetic model to explain multiple peaks in plasma concentration profile of an anticancer drug regorafenib	October 24 (Tue)	16:15-17:00
P07-08☆	Shoma Ito	Kyoto University	Exploring Chemical Structural Insights of ADME Properties via Interpretable Deep Learning	October 25 (Wed)	15:30-16:15
P07-09☆	Kei Kinoshita	Graduate School of Pharmaceutical Sciences, Nagoya City University	Establishment of *in silico* prediction model for skin sensitization aiming for practical application	October 25 (Wed)	16:15-17:00
量子構造生命科学/Computer-Aided Drug Design Quantum-Structural Life Science/Computer-Aided Drug Design					
P08-01☆	Victoire M. L. Cachoux	Iktos	Structure-guided de novo drug design using deep generative modeling: Discovery of a new lead series in only 3 DMTA cycles	October 24 (Tue)	15:30-16:15
P08-02	Shota Uehara	Shionogi & Co., Ltd.	An Approach to Hit Compound Discovery in Shionogi: Ultra-Large Scale Virtual Screening of Synthesizable Compound Libraries.	October 24 (Tue)	16:15-17:00
P08-03	Masao Fujisawa	Kindai University	Solvation Gibbs energies of cyclodextrins	October 25 (Wed)	15:30-16:15
P08-04	Yoshirou Kimura	MOLSIS Inc.	In silico protein design based on genetic algorithm	October 25 (Wed)	16:15-17:00
P08-05	Kyosuke Tsumura	FUJIFILM Corporation	Molecular design method of cyclic peptide inhibitors with cell membrane permeability, and its application to the development of MDMX-p53 inhibitor	October 24 (Tue)	15:30-16:15
P08-06☆	Nozomu Yamazaki	Tokyo Institute of Technology	Improvement of ligand binding affinity prediction based on fair dataset partitioning by bias reduction	October 24 (Tue)	16:15-17:00
P08-07☆	Yudai Araragi	Faculty of Pharmacy, Kanazawa University	Physiologically based pharmacokinetic model describing disposition after repeated oral ingestion of ergothioneine, a food-derived amino acid with neurogenesis activity	October 25 (Wed)	15:30-16:15
P08-08	Masatake Sugita	Tokyo Institute of Technology	Evaluation of the ability of 3D-RISM theory to identify the correct binding mode of small molecule ligands	October 25 (Wed)	16:15-17:00
P08-09☆	Masahito Ohue	Tokyo Institute of Technology	Design of cyclic peptides targeting protein-protein interactions using AlphaFold	October 24 (Tue)	15:30-16:15
P08-10☆	Ryota Ishizawa	Tokyo Institute of Technology	PROTAC molecular linker design using fragment linking method	October 24 (Tue)	16:15-17:00
P08-11	Shigeru Sakurai	bitBiome, Inc.	Efficient enzyme discovery from microbial gene databases and molecular surface features of 3D structures	October 25 (Wed)	15:30-16:15

P08-12☆	Kosuke Maruyama	National Cancer Center Research Institute	Development of a 3D-structure-based drug response model to help annotating kinase mutations for precision medicine	October 25 (Wed)	16:15-17:00
P08-13☆	Daiki Odajima	Hoshi University	Evaluation of binding properties between metabolic glutamate receptor 5 and ligand using fragment molecular orbital method	October 24 (Tue)	15:30-16:15
P08-14☆	Keinoshin Togashi	Tokyo Institute of Technology	Docking prediction of cyclic peptide-protein complex by AlphaFold Multimer with cyclic offset	October 24 (Tue)	16:15-17:00
P08-15☆	Takumi Hirao	University of Tsukuba	Application of Parallel Cascade Selection Molecular Dynamics for generating virtual screening models	October 25 (Wed)	15:30-16:15
P08-16	Yifan Hu	Wuxi Biortus Biosciences Co., Ltd.	Cryo-EM structures of mitochondrial ABC transporter ABCB10 in apo and biliverdin-bound form	October 25 (Wed)	16:15-17:00
バイオインフォマティクス Bioinformatics					
P09-01☆	Mari Nogami Itoh	National Institute of Biomedical Innovation, Health and Nutrition	Integrated network analysis combining EV’s proteomics and serum/urine metabolomics to explore IPF-specific pathways	October 24 (Tue)	15:30-16:15
P09-02☆	Kazuma Hamada	Faculty of Pharmaceutical Sciences, Teikyo Heisei University	Identification of upstream factors that regulate susceptibility to drug-induced mitochondrial toxicity in NAFLD	October 24 (Tue)	16:15-17:00
P09-03☆	Yi-An Chen	National Institutes of Biomedical Innovation, Health and Nutrition	Development of a large-scale database for microbiome and phenotypic data	October 25 (Wed)	15:30-16:15
P09-04☆	Ayaka Mae	Osaka University Graduate School of Information Science and Technology	A Graph Based Method of Pattern Mining for Spatial Transcriptome Data	October 25 (Wed)	16:15-17:00
P09-05	Takashi Amisaki	Tottori University	Using Inter/Intra-Ensemble Variability for Exploring Dynamics and Heterogeneity of Protein Conformations	October 24 (Tue)	15:30-16:15
P09-06☆	Chiharu Konda	OpenEye, Cadence Molecular Sciences	AbXtract™ in Orion -Antibody Discovery in the Cloud-	October 24 (Tue)	16:15-17:00
P09-07☆	Marina Kawai	Genedata KK	A New Workflow Automating Data Analysis in Gene Expression Screens Across Assay Formats Produces Consistent Results at Scale and Efficiency	October 25 (Wed)	15:30-16:15
P09-08☆	Satsuki Ueta	Graduate School of Informatics, Tokyo University of Information Sciences	Application of a doc2vec-based machine learning method toward more reliable prediction of human protein-protein interactions	October 25 (Wed)	16:15-17:00
P09-09	Minae Kawashima	Research Organization of Information and Systems (ROIS)	Toward the development of an information infrastructure to realize a medical examination room with genome information	October 24 (Tue)	15:30-16:15
P09-10	Yosuke Kawai	National Center for Global Health and Medicine	MGeND: A genetic variant database for genomic medicine	October 24 (Tue)	16:15-17:00
臨床インフォマティクス Clinical Informatics					
P10-01	Kohtaro Yuta	In Silico Data,Ltd.	A study on the relationship between "autonomous research" and large-scale generative AI	October 25 (Wed)	15:30-16:15
P10-02	Naofumi Seira	MOLSIS Inc.	Predicting indications of existing drugs for different diseases	October 25 (Wed)	16:15-17:00
P10-03☆	Yohey Kamijo	Nagoya University	Automatic biomarker discovery for idiopathic pulmonary fibrosis by correlation analysis of serum extracellular vesicles proteomic data and clinical data	October 24 (Tue)	15:30-16:15
P10-04☆	Satoshi Mizuno	Tohoku University	Establishment of the precise early prediction models of low-birth-weight for term and preterm birth groups based on genetic and environmental factors	October 24 (Tue)	16:15-17:00
P10-05☆	Okubo Ryosuke	Kampo Medicine Pharmacology Research Laboratory, Graduate School of Pharmaceutical Sciences, Yokohama University of Pharmacy	Exploring the mechanism of action of *Scutellaria baicalensis* for treating pulmonary fibrosis using network pharmacology and molecular docking	October 25 (Wed)	15:30-16:15
P10-06	Soichi Ogishima	Tohoku University	Development of Biobank Network for Research and Development of Precision Medicine in Japan	October 25 (Wed)	16:15-17:00
P10-07☆	Hibiki Mori	Tokyo Institute of Technology School of Life Science and Technology	The relationship between Sessile serrated adenoma/polyp and intestinal bacteria	October 24 (Tue)	15:30-16:15
P10-08☆	Tatsuki Yamamoto	Kyoto university	Elucidation of Mortality Triggers Using Temporal Predictive Models	October 25 (Wed)	15:30-16:15