

演題登録 番号 No.	発表番号 P-No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation	発表時間 Presentation Time
5004	P06-01	Jiaxin Li	The University of Tokyo	Cell State Analysis of Immune Cells in the Tumor Microenvironment with Deep Learning	(A)
5005	P03-01	Daiki Sakai	Yamada Lab, Tokyo Institute of Technology School of Life Science and Technology	Disease Prediction from Small Sample Gut Microbiome Data	(A)
5008	P01-01	YAXUAN WANG	Kagoshima University	Hepatitis C Virus Drug Resistance Mechanism: Docking and Molecular Dynamics Study of NS5A-Drug Complex	(A)
5009	P03-02	Zi Wang	IPR, Osaka Univ.	Biological Age Prediction Using a Deep Neural Network Based on Steroid Metabolic Pathways	(B)
5010	P05-01	Harutoshi Kato	Mitsubishi Tanabe Pharma Corporation	Multi-Task Deep Learning using Graph Convolutional Networks for Predicting the Unbound Fraction in Human, Mouse, and Rat Plasma	(A)
5011	P05-02	Yuki Doi	Mitsubishi Tanabe Pharma Corporation	Enhancing the Reliability of Machine Learning Predictions through Quantitative Evaluation of the Applicability Domain: A Case Study of Multi-Task Prediction Model of Unbound Fraction in Human, Mouse, and Rat Plasma	(B)
5014	P02-01	Hajime Sugiyama	Mitsubishi Chemical Corporation	Investigation of the Allosteric Binding Sites of ERK2 by Metadynamics Simulation	(A)
5015	P06-02	JUNSOO SONG	Institute for Protein Research, Osaka University	A Novel Endometrial Cancer Patient Stratification Considering ARID1A Protein Expression and Function with Effective Use of Multi-omics Data	(B)
5016	P07-01	Toshiaki Watanabe	DAIICHI SANKYO CO., LTD.	Development of Pre-Fragment-Based MMP Analysis	(A)
5017	P07-02	Yasunobu Yamashita	Osaka University	Discovery of a new histone deacetylase 8 inhibitor using machine learning-aided drug screening	(B)
5018	P03-03	Kouki Maebara	Nagoya City University	A deep learning model for predicting chemical-induced rat hepatocellular necrosis using transcriptome data.	(A)
5019	P07-03	Kiyoshi Hasegawa	TECHNOPRO R&D company	Open Source Program Github and Its Application in Drug Discovery	(A)
5020	P03-04	Shogo Nakamura	Tokyo Institute of Technology	Reaction-Aware Molecular Optimization Using Conditional Transformer and Reinforcement Learning	(B)
5023	P03-05	Seiji Matsuoka	RIKEN	Computational determination of SMARTS molecular query containment relationships	(A)
5024	P01-02	Yoshiki Yugami	the department of science, Osaka Prefecture University	Generation of Structural Ensemble of Linear Diubiquitin Based on PCS Experiments	(B)
5025	P07-04	Hiroto Terada	Graduate School of Science, Osaka Metropolitan University	Development of accurate <i>in silico</i> screening protocol based on protein structural fluctuation and drug binding mode	(B)
5026	P07-05	Masatake Sugita	Institute of Science Tokyo	Development of Prediction Models for Membrane Permeability of Cyclic Peptides using 3D Descriptors obtained from Molecular Dynamics Simulations and 2D Descriptors	(A)
5027	P07-06	Yuki Murakami	Yokohama City University	<i>De novo</i> PROTAC linker design to enhance cell membrane permeability based on a data-driven method	(B)
5028	P05-03	Masataka Kuroda	National Institutes of Biomedical Innovation, Health and Nutrition	Development of tools to enhance the extracting process of ADME activity information from the Common Technical Document (CTD)	(A)

演題登録 番号 No.	発表番号 P-No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation	発表時間 Presentation Time
5030	P07-07	Yunoshin Tamura	Preferred Networks	Scaling up Binding Free Energy Calculations: Integrating Free Energy Perturbation (FEP) and Active Learning to Prioritize Compound Designs	(A)
5031	P11-01	Kosuke Takeuchi	DAIICHI SANKYO CO., LTD.	Evaluation of Data-Driven Drug Discovery Approaches: Utilizing Redmine Ticket Management System for Tracking and Analyzing Activities	(B)
5032	P02-02	Kairi Furui	Institute of Science Tokyo	PairMap: An Intermediate Insertion Approach to Improve Accuracy in Relative Free Energy Perturbation Calculations of Distant Compound Transformations	(B)
5033	P07-09	Daiki Ishimoto	Laboratory of Chemistry and Biology, Graduate School of Pharmaceutical Sciences, The University of Tokyo	Development of a Massive Fluorogenic Probe Library Based on Bayesian Optimization toward the Discovery of Novel Biomarker Enzymes	(A)
5034	P11-02	Chihiro Higuchi	National Institutes of Biomedical Innovation, Health and Nutrition (NIBIOHN)	Japanese Food Ontology Development	(A)
5035	P01-03	Chisato Kanai	INTAGE Healthcare Inc.	Investigation of the utility of steered MD in the prediction of binding affinity: a case study of HSP90	(A)
5036	P05-04	ELPRI EKA PERMADI	Institute for Protein Research, Osaka University, Japan	Improving the performance of prediction models for small datasets of cytochrome P450 inhibition with deep learning	(B)
5037	P05-05	Sumie Tajima	HULINKS Inc.	Addressing Common Metabolism Problems in Drug Discovery with <i>in Silico</i> Methods	(A)
5039	P03-06	Takayuki Serizawa	Daiichi Sankyo Co., Ltd.	Development of New data analysis platform for medicinal chemist in Daiichi Sankyo	(B)
5040	P09-01	Ryota Sugie	Mie University	Modular photostable fluorescent DNA blocks for tracking collective movements of motor proteins	(A)
5042	P01-04	Ao Kikuchi	Yokohama City University	Cross-reactivity of T cell receptors against HCoV through three-dimensional structure prediction	(B)
5043	P03-07	Kei Yoshida	Hitachi, Ltd.	Data augmentation method of chimeric protein sequences for fine-tuning of protein language models	(A)
5044	P06-03	Xingran Wang	Institute for Protein Research, Osaka University	Single-Cell Transcriptome Analysis Reveals Roles of GABA Receptors in the Connectivity of Dorsal-Ventral Motor Neurons in <i>C. elegans</i>	(A)
5045	P09-02	Ryosuke Iinuma	JSR Life Sciences Corporation	Size-Selective Capturing of Exosomes Using DNA Tripods	(B)
5047	P01-05	Shoya Hamaue	Daiichi Sankyo Co., Ltd.	Prediction Method for Protein-Bound Conformation of Macrocycles	(A)
5048	P05-06	Ryoko Terada	Institute for protein research of Osaka University	In silico prediction of total clearance, volume of distribution, and half-life with deep learning	(B)
5049	P11-03	Kyosuke Kimura	Meiji Pharmaceutical University	Weibull Analysis of Time-to-Event Patterns in Drug-Induced Liver Injury Associated with Kampo Medicines and Crude Drugs: Insights from the Japanese Adverse Drug Event Report Database	(A)
5050	P06-04	Yulong Gou	Osaka University, Institute for Protein Research	Impact of Intramolecular Hydrogen Bonds on Permeability Glycoprotein Mediated Transportation	(B)
5051	P07-10	Ziwei Zhou	Institute for Protein Research, Osaka University	Virtual validation and the efficient learning methods exploration in federated learning (FL) for drug development research	(B)

演題登録 番号 No.	発表番号 P-No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation	発表時間 Presentation Time
5052	P01-06	Seiya Tanaka	Department of Applied Physics, Graduate School of Engineering, Nagoya University	Enhanced Prediction of Antigen-Antibody Complex Structures through Aggressive Structural Refinement by AlphaFold2	(B)
5053	P07-11	Naoko Konami	Graduate School and School of Pharmaceutical Sciences, Osaka University	Structure and Interaction Analysis of Nucleic Acid Encapsulated ssPalm Lipid Nanoparticles by Multiscale Simulation.	(A)
5054	P06-05	Chaowen Ou	Tokyo Institute of Technology	Improved Method of Predicting Protein Allosteric Site Based on Atomistic Bond-to-bond Interaction by Using GNN	(A)
5057	P01-07	Takashi Yoshidome	Department of Applied Physics, Graduate School of Engineering, Tohoku University	Deep-Learning model for Predicting the Replacement of Water Molecule upon Ligand Binding	(A)
5060	P07-12	Mio Yokoyama	Kumamoto University	Natural-Product Screening Toward Discovery of Anti-Aging Glutaminase-1 Inhibitors. An Electronic-Structure Informatics Study	(B)
5063	P01-08	Hirohata Kaneshiro	Department of Systems Informatics, Graduate School of Systems Informatics, Kobe University	Comprehensive docking simulations using AlphaFold2-based human olfactory receptors for odor prediction	(B)
5064	P09-03	Chung Wing Chan	Graduate School of Science, Kyoto University	Anisotropic Swarming of DNA Modified Microtubules Under UV Light	(A)
5065	P03-08	Yuya Koide	Yokohama National University	Predicting Chemical Roles Using Natural Language Processing on Database Descriptions	(B)
5066	P04-01	Ruri Mihata	Osaka University	Analysis of Kinase Binding Specificity of Staurosporine using the Fragment Molecular Orbital Method	(A)
5068	P07-13	Masami Sako	Tokyo Institute of Technology	DiffInt: Integrating Explicit Hydrogen Bond Modeling into Diffusion Models for Structure-Based Drug Design	(A)
5069	P03-09	Supakorn Pongpakdee	Osaka University	Large-scale single nucleus RNA-seq analysis of Lewy body diseases subtypes	(A)
5070	P01-09	Shinji Iida	Kitasato University	Generative Model for Protein Structural Ensembles Enhanced by Molecular Dynamics Simulation Data	(A)
5071	P08-01	Hiroki Adachi	Chugai Pharmaceutical Co., Ltd.	Predicting clinical laboratory test result related to urine tests in patients with chronic kidney disease	(A)
5072	P02-03	Siyun Wang	Graduate school, Osaka university	Fragment Molecular Orbital Calculations for Zinc-Containing smHDAC8	(A)
5074	P07-14	Keisuke Yanagisawa	Tokyo Institute of Technology	QUBO Problem Formulation of Fragment-Based Protein-Compound Flexible Docking	(B)
5075	P07-15	Kaho Akaki	Institute of Science Tokyo	Acquisition of Bias Information for Protein-Ligand Docking by Mixed-Solvent Molecular Dynamics	(A)
5076	P07-16	Shimizu Masayoshi	Institute of Science Tokyo	Development of a compound pre-screening method based on docking of fragments	(B)
5077	P02-04	Suzu Itami	Kindai University	Interaction Analysis between pHLA and TCR using MD Simulation and Fragment Molecular Orbital Calculation	(B)
5079	P01-10	Toshiaki UEDA	Graduate School of Science and Technology, Shinshu University	Epicatechin n -mers ($n \geq 5$) adopt more compact conformations than catechin n -mers	(B)
5080	P02-05	Junya Yamagishi	Preferred Networks	NNP-based Force Field Optimization to Improve RBFEP Performance	(A)

演題登録 番号 No.	発表番号 P-No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation	発表時間 Presentation Time
5081	P03-10	Hiroyuki Hakamata	Daiichi Sankyo Co., Ltd.	SAR analysis and visualization utilizing a fragment-based approach: Application to a public data analysis of Targeted Protein Degradation	(B)
5082	P01-11	Takunori Yasuda	Institute of Life and Environmental Sciences, University of Tsukuba	The Computational Study on the Secondary Structure Formation of Nascent Peptides Inside the Ribosome Tunnel with Biomolecular Environments Mimicking Model	(A)
5083	P03-11	Jianan Li	Institute of Science Tokyo	CycPeptMP: Development of Membrane Permeability Prediction Model of Cyclic Peptides with Multi-Level Molecular Features and Data Augmentation	(A)
5084	P07-17	Yuma Iwashita	Laboratory of Medical Molecular Analysis, Meiji Pharmaceutical University	Report on Participation in the Tox24 Challenge: Construction of a High-Accuracy QSAR Predictive Model for Transthyretin Activity	(A)
5085	P09-04	Hisashi Tadakuma	ShanghaiTech University	De novo protein design of suitable binders for DNA origami-based devices	(B)
5086	P03-12	Keisuke Hirota	Institute of Science Tokyo	Deep learning-based enzyme screening to identify orphan enzyme genes	(B)
5087	P07-18	Taiyo Toita	Yokohama City University	Lead generation of a V-ATPase inhibitor using molecular generative AI	(B)
5089	P07-19	Yifan Hu	Biotus Biosciences Co. Ltd	Exploring the Power of Structural Biology on Degradation Discovery	(A)
5091	P11-04	Kiyohiro Toyofuku	Kyushu University	Development of a model to predict the severity of systemic lupus erythematosus using LIFE Study data	(B)
5094	P03-13	SAID BYADI	HOKKAIDO UNIVERSITY	Data-driven design of visible-light photoswitches using structural features	(A)
5095	P06-06	Yuki Kobayashi	Kyoto University	Development of RNA velocity method using numerical integration of ordinary differential equations	(B)
5096	P07-20	Kentaro Kawai	Setsunan University	Constructing a machine learning model for discriminating Urotensin-II receptor inhibitors and its application	(B)
5099	P03-14	Kikuko Kamisaka	RIKEN	Recent Developments of FMO in 2024: Efforts Towards Utilization of FMO data	(B)
5100	P03-15	Miwa Sato	Hitachi, Ltd	Development of the data management system to acquire the strategic data for AI	(A)
5101	P07-21	Apakorn Kengkanna	Institute of Science Tokyo	Reaction-conditioned variational autoencoder model for catalyst generation and catalytic performance prediction	(A)
5102	P04-02	Shuhei Miyakawa	Osaka University	Dynamical Interaction Energy Analysis of Elastase in Each Reaction State: Insights from Molecular Dynamics and Fragment Molecular Orbital Calculations	(B)
5103	P02-06	WENXING HU	Tokyo Institute of Technology	SpatialPPI 2.0: Enhancing Protein-Protein Interaction Prediction Through Distance Matrix Analysis Using Link Regression in Graph Attention Networks	(B)
5105	P03-16	Yi-An Chen	National Institutes of Biomedical Innovation, Health and Nutrition	Enhancing Biological Insights with TargetMine: Integration of Genomic Region Annotations	(B)
5106	P04-03	Jun Koseki	National Institute of Advanced Industrial Science and Technology	Development of the Cryptic Site searching method with Mixed-solvent molecular dynamics and Topological data analyses methods	(A)
5108	P08-02	Shoki Hoshikawa	Faculty of Pharmaceutical Sciences, Setsunan University	Machine learning models for predicting cross-reactivity of beta-lactam antibiotic allergy	(B)

演題登録 番号 No.	発表番号 P-No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation	発表時間 Presentation Time
5109	P01-12	Kei Terakura	Institute of Science Tokyo	Kinetic Analysis of Membrane Permeation Process of Cyclic Peptides Using Markov State Models with Molecular Dynamics Simulations	(B)
5110	P03-17	Koh Sakano	Institute of Science Tokyo	Natural product-like compound generation with chemical language models	(A)
5111	P03-18	Tsubasa Nagae	Yokohama City University	Development of an Integrated Machine Learning Model Incorporating Compound-Protein Information for Design and Prediction of Small-Molecule Modulators of PPIs	(B)
5112	P02-07	Xingmei Ouyang	RIKEN	Development of RIKEN Natural Products Depository Database	(A)
5113	P11-05	Kaito Sasaki	Kyushu University	Exploring unexpected factors related to glaucoma onset in diabetes patients using LIFE Study data	(A)
5115	P01-13	Osamu Ichihara	Schrödinger KK	Predicting Lysine Reactivity: Insights from Constant-pH MD Simulations and Experimental Correlation	(A)
5116	P10-01	Yunosuke Matsuda	Bathclin Corporation	Decision-making model to enhance subjective well-being through individualized lifestyle modifications based on counterfactual explanation	(A)
5117	P07-22	KOSUKE MINAGAWA	Daiichi Sankyo Co., Ltd.	Drug discovery research utilizing BROOD: A Fragment Replacement and Molecular Design tool	(B)
5120	P02-09	Yurika Ikegami	University of Tsukuba Graduate School	Computational assessment of the binding mode of Verteporfin, an inhibitor targeting the YAP-TEAD protein-protein interaction	(A)
5122	P03-19	Toru Nishino	FUJIFILM Corporation	REALM: Region-Empowered Antibody Language Model for Antibody Property Prediction	(A)
5123	P03-20	Daiki Koge	Niigata University	Generalized Molecular Representation for Drug Discovery via Molecular Graph Latent Diffusion Autoencoder	(B)
5124	P07-23	Sora Suzuki	International Graduate Program for Agricultural and Biological Science Selection	A small molecule inhibitor that binds to the unstable state of its target kinase DYRK1A demonstrates slowly dissociation from the complex	(A)
5128	P03-21	Toshiyuki Ohfusa	Astellas Pharma Inc.	Data utilization and DX talent development on in-house KNIME platform	(A)
5129	P07-24	Yoshiro Kimura	MOLSIS Inc.	Correlation Analysis of Excipient Modulated Viscosity of Monoclonal Antibody and Molecular Surface Patch Properties	(B)
5131	P04-04	Katsuki Sato	Department of Chemistry, Tokyo University of Science	Analysis of HS-AFM images of proteins combining MD simulation and machine learning	(B)
5132	P01-14	Yuki Yasumitsu	Institute of Science Tokyo	Protein Tertiary Structure Prediction with Fine-tuned AlphaFold2 for Ligand Virtual Screening	(B)
5133	P07-25	Takuya Tsutaoka	FUJIFILM Corporation	Predicting Antibody Stability pH Values from Amino Acid Sequences: Leveraging Protein Language Models for Formulation Optimization	(A)
5136	P03-22	Takanobu Araki	Astellas Pharma Inc.	Astellas's Digital Transformation for Small Molecule Drug Discovery Research	(B)
5137	P01-15	Yoshitaka Tadokoro	KINDAI University	Dynamic Relationship Between the Entrance to the Ligand Binding Site and the Dimer Interface in MAO-B	(A)
5139	P07-26	Okimasa Okada	Mitsubishi Tanabe Pharma Corporation	Development of a Platform for Crystal Structure Prediction of Drug Molecules	(B)
5140	P07-27	Takashi Ikegami	MOLSIS Inc.	Automated molecular modeling and property assessment for ADCs	(A)

演題登録 番号 No.	発表番号 P-No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation	発表時間 Presentation Time
5141	P01-16	Ekishin Yanagi	The University of Tokyo	Conformational study of macrocyclic peptides in solvent by MD simulations to improve their membrane permeability	(B)
5142	P02-10	Kazuya Osumi	Toray Industries, Inc.	Case studies of deep learning-based molecular docking program in medicinal chemistry	(B)
5146	P03-23	Hirokazu Nishimura	Mitsubishi Tanabe Pharma Corporation	Unraveling Microbiome Complexity: A Knowledge Graph Approach to Functional Interpretation in Drug Discovery	(A)
5147	P03-24	Nagisa Matsuo	Kanazawa University	Age prediction from DNA methylation data using machine learning	(B)
5149	P11-06	Hiromu Matsumoto	Kyushu University	Survival Analysis of Chronic Kidney Disease Using Multi-Regional Data from the LIFE Study	(B)
5150	P03-25	Hiromitsu Shimoyama	The Noguchi Institute	Exchange System for Glycan Textual Notations Development to Integrate Various Glycan Databases and Improve Search Accuracy	(A)
5151	P07-28	Tomoki Yonezawa	Keio University	Validation of the reproducibility of hit-to-candidate using ChemTS	(B)
5152	P01-17	Yudai Kobayashi	Department of Biomedical Data Intelligence, Graduate School of Medicine, Kyoto University	High-precision and Efficient Prediction of Intermolecular Interaction Energies Using Deep Learning on Quantum Chemical Calculation Data	(A)
5153	P06-07	Akira Shinohara	Tokyo Institute of Technology	Compound Retrosynthesis Analysis Using Consensus Estimate	(A)
5156	P11-07	Kensei Orita	Kyushu University	Data-driven search for diseases whose patient numbers are associated with weather variability using LIFE study data	(A)
5157	P07-29	Genki Kudo	University of Tsukuba	Automated Hit-to-Lead Optimization Using the SINCHO Protocol and ChemTS	(A)
5158	P03-26	Noriaki Okimoto	RIKEN	Drug discovery study integrating compound generative AI and molecular docking	(B)
5159	P11-08	Ryoji Abe	Tokyo Institute of Technology	Analysis of interactions between fatty acid membranes with pH-dependent phase structures and nucleic acid monomers using Molecular Dynamics simulation	(B)
5160	P02-11	Kodai Igarashi	Institute of Science Tokyo	Binding Affinity Prediction Through Unsupervised Learning of Protein-Ligand MD Trajectories	(A)
5162	P01-18	Hiroaki Oheda	Yokohama City Univ.	Mechanisms of Type-51 R-body conformational changes revealed by in silico methods	(B)
5163	P02-12	Hirofumi Watanabe	WithMetis Co., Ltd.	Preprocessing of FMO calculations and practical visualization of interaction energies for drug design	(B)
5164	P11-10	Kohtarō Yuta	In Silico Data, Ltd.	From Computer-Assisted Routine/Repeated 'Automation' to AI-Assisted Future-Oriented 'Autonomous (Intelligent/Creative)': Division and Impact of 'Automation' and 'Autonomous' in Research Contents	(B)
5165	P07-30	Yuka Matsumoto	Fujifilm Corporation	Application of Amino-Acid Mapping: Activity Prediction for Drug Discovery	(B)
5166	P09-05	Rinka Aoki	Graduate School of Engineering, Tohoku University	Over the Membrane: Study of Nucleic Acid Sequence Transfer Using Cholesterol-Modified DNA	(A)
5167	P02-08	Tomohiro Sato	RIKEN	Machine learning based prediction of quantum mechanical interaction energy between amino acid residues using fragment molecular orbital method	(B)
5168	P06-08	Kohei Hoashi	Tokyo Institute of Technology	Development of docking simulation with high-speed graph neural network scoring function	(B)

演題登録 番号 No.	発表番号 P-No.	氏名 Name	所属 Affiliation	演題名 Title of Presentation	発表時間 Presentation Time
5169	P07-31	Jinzhe Zhang	Preferred Networks Inc	Efficient Single Step Synthesizable Molecular Design using Wasserstein Autoencoder	(A)
5170	P02-13	Ryosuke Kita	Kyushu university	Prediction of quantum mechanical interactions between the ligand and each amino acid residue in protein-ligand complexes	(A)
5171	P06-09	Mao Tanabe	National Institutes of Biomedical Innovation, Health and Nutrition	Investigation of the trends and the potential in drug development for rare and intractable diseases based on the KEGG NETWORK	(A)
5172	P09-06	Yuri Kobayashi	Mie university	Multi-reconfigurable DNA nanolattice guided by a combination of external stimuli	(B)
5173	P01-19	Kenji Yamagishi	Nihon University	Molecular simulation analysis for nucleic acids	(A)
5175	P11-09	Yuhui Zhang	Tokyo Institute of Technology	A Virtual Reality Platform for Molecular Dynamics Based on Unity Engine	(A)
5176	P03-27	Masato Sakagami	Kanazawa University	Spike separation of high-gamma power in ECoG using peak detection	(A)
5177	P06-10	Ryui Sato	Tokyo Institute of Technology	Prediction of medium components for bacteria using deep Learning	(B)
5178	P05-07	Yuki Umemori	Axceed Tokyo West Partners	Unbound Fraction Optimized Method for Predicting Human Pharmacokinetic Clearance: Advanced Allometric Scaling Method and Machine Learning Approach	(A)
5181	P09-07	Ryoya Sakaguchi	Mie University	Construction of dual-responsive circular DNA origami nanoactuator	(A)
5184	P03-28	Masafumi Saito	Kanazawa University	Estimation of transmission routes of the COVID-19 BA.1.1.2 variant using McAN and 3D graph visualization	(B)
5185	P07-32	MARTIN -	Hokkaido University	Quantitative Assessment of Protein-Ligand Activity Prediction from 3D Docking Poses for Urate Transporter 1	(B)
5186	P07-33	Tomoya Saito	Institute of Science Tokyo	Development of an efficient compound 3D conformer search system based on relative position of fragments	(A)
5187	P01-20	Samuel Toba	OpenEye, Cadence Molecular Sciences	Induced-Fit Posing (IFP): A new pose prediction tool for hit to lead stage of drug discovery	(B)
5188	P07-34	Koshiro Aoki	Institute of Science Tokyo	Molecular Properties Prediction by Contrastive Learning Using Graph Neural Network	(B)
5189	P06-11	Koki Hattori	Chiba University	Elucidation of Stabilization Mechanisms of Intrabodies Based on Statistical Thermodynamics	(A)
5191	P09-08	Koichi Tanimoto	Kansai University	Evaluation of anticancer activity and investigation of cellular uptake mechanism of drug-loaded DNA Origami dendrimers for application to drug delivery system	(B)
5193	P01-21	Keisuke Uchikawa	Institute of Science Tokyo	Generation of a suitable structure for SBDD by AlphaFold2 via Genetic Algorithm Parameter Search	(A)
5195	P03-29	Shuto Hayashi	Institute of Science Tokyo	A framework for enhanced de novo protein design using deep learning and bayesian optimization	(A)
5197	P07-08	Koichi Oki	Nagoya University	A Dirichlet diffusion model for generation of high-quality antimicrobial peptide sequences	(B)
5199	P03-30	Yusuke SAKAI	RIKEN	Directional Graph Modelling for Solution Design and Experiment Automation	(B)