Chem-Bio Informatics Society(CBI) Annual Meeting 2022 <Poster List> Poster No. : P-Category-ID

演題登録番号	p-No	Title	First Author	Affiliations	Category	Date of presentation	Time of presentation
5003	P01-01	Cyclosporin A: Conquering Conformational Complexity and Chameleonicity	Satoshi Ono	Mitsubishi Tanabe Pharma Corporation	01.Computational Chemistry (Molecular Modeling)	October 25 (Tue)	17:00-18:00
5010	P01-02	Toward a in silico screening of broad-spectrum antibody that is effective against wide variety of variants	Kanji Oshima	KANEKA CORPORATION	01.Computational Chemistry (Molecular Modeling)	October 25 (Tue)	18:00-19:00
5015	P01-03	Structure prediction of cyclic peptides in solvent with integrating multiple technologies	Kentaro Takai	Fujitsu Ltd	01.Computational Chemistry (Molecular Modeling)	October 26 (Wed)	17:00-18:00
5016	P01-04	Molecular dynamics study of the interaction between a GST dimer and a novel peptidic covalent aptamer	Lisa Matsukura	Graduate school of BOST, KINDAI	01.Computational Chemistry (Molecular Modeling)	October 26 (Wed)	18:00-19:00
5061	P01-05	QM/MM simulations of artificial ion channel in membrane-water system	Mayuko Nakagawa	Yokohama City University	01.Computational Chemistry (Molecular Modeling)	October 25 (Tue)	17:00-18:00
5063	P01-06	Pursuit of elementary reactions by the difference of H/D using the Nuclear-Electronic Orbital method	Kohei Motoki	Chuo University	01.Computational Chemistry (Molecular Modeling)	October 25 (Tue)	18:00-19:00
5077	P01-07	Prediction of Structural Change of siRNA by 2-formamide, a Newly-synthesized Chemical Modification, via Density Functional Theory	Seongjin An	The University of Tokyo	01.Computational Chemistry (Molecular Modeling)	October 26 (Wed)	17:00-18:00
5090	P01-08	Metadynamics simulation of protein-based nanoparticles	Kazutoshi Takahashi	Ajinomoto Co., Inc.	01.Computational Chemistry (Molecular Modeling)	October 26 (Wed)	18:00-19:00
5097	P01-09	Simulation study of the interaction between lipids and the complex structure of γ-secretase and APP or Notch.	Chika Minami	KINDAI Univ.	01.Computational Chemistry (Molecular Modeling)	October 25 (Tue)	17:00-18:00
5104	P01-10	Conformational behavior and dynamics of G7A mutant IgG-aptamer	Seiichiro Ishii	Nihon University	01.Computational Chemistry (Molecular Modeling)	October 25 (Tue)	18:00-19:00
5008	P02-01	Energy decomposition analysis for cyclodextrins-furosemide complexes	Masao Fujisawa	kindai University	02.Computational Chemistry (Molecular Recognition)	October 26 (Wed)	17:00-18:00

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5045	P02-02	Insight into Allosteric ERK2 Inhibitors by using Metadynamics Simulations	Hajime Sugiyama	Mitsubishi Chemical Corporation	02.Computational Chemistry (Molecular Recognition)	October 26 (Wed)	18:00-19:00
5079	P02-03	Interaction analyses of inhibitors against threonyl-tRNA synthetase by fragment molecular orbital calculations	Yoshiharu Mori	Kobe University	02.Computational Chemistry (Molecular Recognition)	October 25 (Tue)	17:00-18:00
5093	P02-04	Amino acid preference mapping on protein-protein interaction surface using mixed-solvent molecular dynamics	Genki Kudo	University of Tsukuba	02.Computational Chemistry (Molecular Recognition)	October 25 (Tue)	18:00-19:00
5099	P02-05	Practical visualization of interaction energies by FMO for drug design	Hirofumi Watanabe	WithMetis Co., Ltd.	02.Computational Chemistry (Molecular Recognition)	October 26 (Wed)	17:00-18:00
5004	P03-01	Investigation of the applicability domain for prediction model using in-house data	Toshiaki Watanabe	DAIICHI SANKYO CO., LTD.	03.Data Science	October 26 (Wed)	18:00-19:00
5013	P03-02	Deep Learning for Cellular Morphological Change Detection with High Throughput Images	Yuko Nirei	Mitsubishi Tanabe Pharma Corporation	03.Data Science	October 25 (Tue)	17:00-18:00
5019	P03-03	Investigation of the relationship between the performance of Encoder-Decoder model and the characteristic of molecular representation obtained	Shumpei Nemoto	The University of Tokyo	03.Data Science	October 25 (Tue)	18:00-19:00
5022	P03-04	Integrated browsing of chemical reactions registered in Electronic Lab Notebook and external data	Yu Endo	Nippon shinyaku co., ltd.	03.Data Science	October 26 (Wed)	17:00-18:00
5027	P03-05	Construction D4 environment for Patent informatics	Takayuki Serizawa	DAIICHI SANKYO CO.,LTD.	03.Data Science	October 26 (Wed)	18:00-19:00
5034	P03-06	Estimation of amino-acid interaction potentials with structure similarity calculated by Digital Annealer	Chieko Terashima	Fujitsu Limited.	03.Data Science	October 25 (Tue)	17:00-18:00
5035	P03-07	Recent developments of FMODB: enhancement of the IFIE/PIEDA interface for analyzing the related FMO calculation data of bio-macromolecules	Kikuko Kamisaka	RIKEN Center for Biosystems Dynamics Research	03.Data Science	October 25 (Tue)	18:00-19:00
5040	P03-08	Reservoir Computing for Efficient Prediction of Optical Response of Digital Metamaterial	Tomoya Meguro	Okayama University	03.Data Science	October 26 (Wed)	17:00-18:00

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5051	P03-09	Assessment of iterative screening for drug discovery using an unbiased dataset	Akira Kimura	RIKEN	03.Data Science	October 26 (Wed)	18:00-19:00
5052	P03-10	Constructing a systematic knowledge graph using real-world data	Takeshi Takagi	EPS Corporation	03.Data Science	October 25 (Tue)	17:00-18:00
5078	P03-11	Proposal and Outline of the “Autonomous Chemistry” Research	Kohtaro Yuta	In Silico Data,Ltd.	03.Data Science	October 25 (Tue)	18:00-19:00
5080	P03-12	Protein-ligand complex structure generation with diffusion-based generative models	Shuya Nakata	Kobe University	03.Data Science	October 26 (Wed)	17:00-18:00
5088	P03-13	Development of a method for building a long-term disease progression model using neural networks	Ryota Jin	Chiba University	03.Data Science	October 26 (Wed)	18:00-19:00
5062	P04-01	Computational search for compounds exhibiting the same activity from database by molecular fingerprints and 3D pseudo-atom methods	Mizuki Matsushita	Shinshu University	04.Structure Activity Relationship	October 25 (Tue)	17:00-18:00
5089	P04-02	Analysis of protein-protein dynamical interaction by molecular dynamics and principal component analysis	Keima Kawada	Nihon University	04.Structure Activity Relationship	October 25 (Tue)	18:00-19:00
5102	P04-03	Constructing QSAR models for c-Met inhibitors	Yu-Shi Tian	Osaka University	04.Structure Activity Relationship	October 26 (Wed)	17:00-18:00
5094	P05-01	Molecular Evolution of Peptides and Energy Level Statistics of Dipeptides and Tripeptides	Masanori Yamanaka	Nihon University	05.Quantum-Structural Life Sscience	October 26 (Wed)	18:00-19:00
5107	P05-02	KEK GoToCloud project: An Application of Cloud Computing for Structural Biology Research in KEK	Yusuke Yamada	High Energy Accelerator Research Organization	05.Quantum-Structural Life Sscience	October 25 (Tue)	17:00-18:00
5014	P06-01	Prediction of drug-induced liver injury in silico using large-scale adverse event database	Sarara Doi	Graduate School of Pharmaceutical Sciences, Nagoya City University	06.ADMET	October 25 (Tue)	18:00-19:00
5046	P06-02	Characterizing Predictive Effects of Autophagy Agents on the Early Stages of Embryo Development	Kengo Matsuba	Yokohama University Pharmacy	06.ADMET	October 26 (Wed)	17:00-18:00

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5069	P06-03	Application of Deep Learning to the Evaluation of Seizure-like Behavior Using Zebrafish	Mizuho Wakasa	Otsuka Pharmaceutical Co., Ltd.	06.ADMET	October 26 (Wed)	18:00-19:00
5065	P07-01	Artificial Intelligence to Accelerate New Drug Discovery: Target identification and drug discovery by data-driven approach and experimental validation in Idiopathic Pulmonary Fibrosis (IPF)	Mari Itoh	National Institute of Biomedical Innovation, Health and Nutrition	07.Bioinformatics	October 25 (Tue)	17:00-18:00
5101	P07-02	Five cluster groups found in the health state space of 96,093 population	Satoshi Nagaie	Tohoku Medical Megabank Organization, Tohoku University	07.Bioinformatics	October 25 (Tue)	18:00-19:00
5002	P08-01	Proposal of a simple pose descriptor for prediction of correct docking poses by machine learning approaches	Kentaro Kawai	Setsunan University	08.Drug Discovery Application	October 26 (Wed)	17:00-18:00
5005	P08-02	Global Assessment of Substituents on the Basis of Analogue Series	Kosuke Takeuchi	DAIICHI SANKYO CO., LTD.	08.Drug Discovery Application	October 26 (Wed)	18:00-19:00
5020	P08-03	Validation of low-resolution protein crystal structures using deep learning	Takaaki Kuribayashi	Mitsui Knowledge Industry Co., LTD	08.Drug Discovery Application	October 25 (Tue)	17:00-18:00
5026	P08-04	Improvement of Compound-Protein Interactions Prediction with Semi-Supervised Learning	Takuto Koyama	Graduate School of Medicine, Kyoto University	08.Drug Discovery Application	October 25 (Tue)	18:00-19:00
5031	P08-05	Search for allosteric chaperones for lysosomal acid α-glucosidase	Manami Yamazaki	Graduate School of Pharmacieutical Science, Kitasato University	08.Drug Discovery Application	October 26 (Wed)	17:00-18:00
5037	P08-06	Prediction of pharmacological activity by deep learning using skeletal formula images	Satoshi Ito	Digital Hollywood University graduate school	08.Drug Discovery Application	October 26 (Wed)	18:00-19:00
5043	P08-07	AI-AAM. Downsizing and scaffold hopping from a peptide to small-molecule inhibitors	Shino Ohira	Fujifilm corporation	08.Drug Discovery Application	October 25 (Tue)	17:00-18:00

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5053	P08-08	Graph based property and affinity prediction using open-source tool and cloud platform	Akitoshi Okada	JAPAN TABACCO INC.	08.Drug Discovery Application	October 25 (Tue)	18:00-19:00
5064	P08-09	Development of a screening system for RNA-binding small molecules based on large-scale information of interactions between RNAs and a fluorescence indicator	Ryosuke Nagasawa	IMRAM Tohoku Univ.	08.Drug Discovery Application	October 26 (Wed)	17:00-18:00
5070	P08-10	Reducing the Data Bias in the PDBbind Database	Nozomu Yamazaki	Department of Computer Science, Tokyo Institute of Technology, Ishida Laboratory	08.Drug Discovery Application	October 26 (Wed)	18:00-19:00
5072	P08-11	Estimation of Interaction Mechanism in Compound-Protein Interaction Prediction Using Interpretable Deep Learning	Sota Inoue	Kyoto University	08.Drug Discovery Application	October 25 (Tue)	17:00-18:00
5073	P08-12	Lead optimization through active learning using free energy perturbation	Kairi Furui	Tokyo Institute of Technology	08.Drug Discovery Application	October 25 (Tue)	18:00-19:00
5075	P08-13	Prediction of Class A GPCR-Compound interactions by deep learning focusing on ligand binding site protein sequences	Haruki Yamane	Tokyo Institute of Technology	08.Drug Discovery Application	October 26 (Wed)	17:00-18:00
5083	P08-14	AI-AAM. Lead-to-lead scaffold hopping for drug repositioning	Jun Nakabayashi	FUJIFILM Corporation	08.Drug Discovery Application	October 26 (Wed)	18:00-19:00
5086	P08-15	Understanding Molecular Mechanism of Drug Off-Target Effect in Tyrosine-Protein Kinase LCK Using Molecular Dynamics Simulation	Hidetoshi Tage	Department of Biomedical Data Intelligence, Graduate School of Medicine and Faculty of Medicine, Kyoto University	08.Drug Discovery Application	October 25 (Tue)	17:00-18:00
5100	P08-16	Molecular Generation for Protein-Protein Interaction Inhibitor Design focusing on Physicochemical Properties	Yuki Kojima	Tokyo Institute of Technology	08.Drug Discovery Application	October 25 (Tue)	18:00-19:00

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5103	P08-17	Multi-objective Bayesian optimization for antimicrobial peptides design using non-natural amino acids	Yuki Murakami	Yokohama City University	08.Drug Discovery Application	October 26 (Wed)	17:00-18:00
50002	P08-18	Automated design of novel drugs using patent literature	András Strácz	Patcore, Inc,	08.Drug Discovery Application	October 26 (Wed)	18:00-19:00
50007	P08-19	Automated hetero shuffling combined with FMO calculations	Sundaram Arulmozhiraja	Asahi Kasei Pharma	08.Drug Discovery Application	October 25 (Tue)	17:00-18:00
50008	P08-20	In Silico Identification of Natural Product Compounds as a Selective Endoplasmic Reticulum α-Glucosidase II Inhibitors using Pharmacophore-based Virtual Screening and Molecular Docking Studies	Mochammad Nasution	Osaka University	08.Drug Discovery Application	October 25 (Tue)	18:00-19:00
5028	P10-01	Gentamicin-induced hearing loss: a retrospective study using the Food and Drug Administration Adverse Event Reporting System and a drug−gene network analysis using the DIseAse MOdule Detection algorithm	Mitsuhiro Nakamura	Gifu Pharmaceutical University	10.Regulatory Science	October 26 (Wed)	17:00-18:00
5049	P10-02	Comprehensive analysis of the drugs that may induce severe cutaneous adverse reactions using the adverse drug event report database	Risa Tonegawa	Meiji Pharmaceutical University	10.Regulatory Science	October 26 (Wed)	18:00-19:00
5082	P10-03	Development of Prediction Model for Adverse Events by Using Spontaneous Report Database and Chemical Structures	Keiko Ogawa	Ritsumeikan University	10.Regulatory Science	October 25 (Tue)	17:00-18:00
5066	P11-01	Analysis of Ion Transport Properties in Artificial DNA Channels with Molecular Dynamics	Jun Takahashi	SCHOOL OF ENGINEERING, TOHOKU UNIVERSITY	11.Molecular Robotics	October 25 (Tue)	18:00-19:00
5084	P11-02	Luminescent control of DNA-scaffolded BRET system using strand displacement reaction	Fumiaki Takano	Kansai University	11.Molecular Robotics	October 26 (Wed)	17:00-18:00
5085	P11-03	Long-range and multi-step intramolecular energy transfer by BRET/FRET system	Yuki Minamide	Kansai University	11.Molecular Robotics	October 26 (Wed)	18:00-19:00

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5009	P12-01	Predicting Excipient Modulated Viscosity of Monoclonal Antibody Formulations	Yoshirou Kimura	MOLSIS Inc.	12.Modality	October 25 (Tue)	17:00-18:00
5011	P12-02	Specific knockdown of KRAS mutant gene using SNPD-siRNA repressed cell proliferation of pancreatic cancer cells in vitro and in vivo	Yoshiaki Kobayashi	Graduate School of Science, The University of Tokyo	12.Modality	October 25 (Tue)	18:00-19:00
5048	P12-03	Development of Precise Genome Editing Technology by Cell Cycle Depending Activation of CRISPR-Cas9	Daisuke Matsumoto	Hiroshima University	12.Modality	October 26 (Wed)	17:00-18:00