演題一覧表 - Cheminformatics

カテゴリー: C1 genome-wide & omics study
C2 SAR, pharmacokinetics
C3 drug design, screening, sorting
C4 molecular dynamics, docking
C5 quantum mechanics, FMO
C6 computing & simulation
C7 medical system & others

ポスター番号	演題	筆頭著者	所属	カテゴリー						
C01_30	Prediction of the complex structure between PI3K and romidepsin (FK-228) for drug design of PI3K/HDAC dual inhibitors	Akifumi Oda	Kanazawa University				C4			
C02_54	Pattern recognition analysis of 1H NMR spectra of plasma and waste-fluid from patients in hemodialysis therapy	Takao Shinkawa	Tohoku University							C7
C03_77	Acceleration of quantum chemistry and chemical similarity calculations on GPGPU architecture towards faster virtual screening	Yuki Furukawa	X-Ability Co. Ltd.					C5		
C04_122	Detection of structural elements which may control transduction pathway of GPCRs based on MD calculation and sequence analysis	Minoru Sugihara	CBRC, AIST				C4			
C05_46	CARCINOscreen®: Novel short term prediction system for carcinogenicity of chemicals by hepatic transcript profiling in a 28-day repeat-dose toxicity study	Fumiyo Saito	Chemicals Evaluation and Research Institute	C1						
C06_51	Establishment of a dose setting method for the CARCINOscreen®: a new short-term chemical carcinogenicity screening method	Hiroshi Matsumoto	Chemicals Evaluation and Research Institute			C3				
C07_143	Structure prediction for proteins screened critically to autoimmune diseases based upon bioimformatics with Isolated-FAMS	Mitsuo Iwadate	Chuo University			C3				
C08_144	Optimization for placement of secondary structures and multiple consensus selection for structures obtained from homology modeling	Takahiro Miyashita	Chuo University				C4			
C09_94	Development of G9a inhibitor using molecular simulations	Yoshinori Hirano	Quantitive Biology Center, RIKEN				C4			
C10_145	Improvement of sampling efficiency through combined use of simulations with implicit and explicit solvent models	Hiroko Kondo	Quantitive Biology Center, RIKEN				C4			
C11_113	Computational design of short peptide inhibitors of protein-protein interactions in intracellular signaling mediated by CRK-SH2	Junya Yamagishi	University of Tokyo				C4			
C12_118	Capturing drug responses by quantitative promoter profiling	Kazuhiro Kajiyama	Omics Science Center, RIKEN		C2					
C13_70	Systematically selected standard set of the substituents for SAR exploration	Noriaki Hashimoto	Systems and Structural Biology Center, RIKEN		C2					
C14_155	Regulation of differentiation via microRNAs controlled by master regulator transcription factors during adipocyte/osteoblast	Yosuke Mizuno	Saitama Medical University	C1						
C15_159	Exome sequencing for the disease-mutation search of mitochondrial respiratory chain	Masakazu Kohda	Saitama Medical University	C1						
C16_161	Exome sequencing and family-based analysis for the identification of a mutation in a Japanese family with Malignant Hyperthermia	Nana Matoba	Saitama Medical University	C1						
C17_164	Id4, a new candidate gene for senile osteoporosis acts as a molecular switch promoting osteoblast differentiation	Yoshimi Tokuzawa	Saitama Medical University	C1						
C18_165	Integrated analysis of non-coding RNAs expression during bi-directional differentiation from mouse mesenchymal stem cells to	Yutaka Nakachi	Saitama Medical University	C1						
C19_21	RNA-sequencing-based screening of functional long non-coding RNAs in MCF7 breast cancer	Kuniko Horie-Inoue	Saitama Medical University	C1						
C20_49	Genome-wide identification of estrogen responsive genes in breast cancer MCF-7 cells using cap analysis of gene expression	Kazuhiro Ikeda	Saitama Medical University	C1						

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C21_53	Identification and characterization of human genomic binding sites for retinoic acid receptor/retinoid X receptor heterodimers	Takatsugu Kosugi	Toho University	C1						
C22_61	Identification of androgen receptor binding sites in the human genome	Akiko Murasaki	Toho University	C1						
C23_80	Identification and characterization of human genomic binding sites for retinoid X receptor	Hiroki Saito	Toho University	C1						
C24_25	Towards a parallel and distributed particle simulation in a cloud computing environment	Akihiro Komorida	Tokyo Institute of Technology						C6	
C25_22	Application of a new global parameter optimization method for analyzing pharmacokinetic drug-drug interactions	Kenta Yoshida	University of Tokyo		C2					
C26_3	An interaction network of biological entities extracted from the literatures on aging studies	Kyoko Hirano	International Medical Information						C6	
C27_12	Frame design and partial implementation of the CADU platform	Tsuguchika Kaminuma	Institute for Cyber Associates							C7
C28_16	A novel method for analyzing protein termini	Taro Kishimoto	Mitsubishi Tanabe Pharma Corp.							C7
C29_60	"Expression trajectories" of reprogramming and differentiation on expression potential field	Tadashi Miyamoto	Tokyo Medical and Dental University							C7
C30_62	A pathway based prioritization for risk genes of bipolar disorder	Hashime Sawai	Tokyo Medical and Dental University						C6	
C31_87	From computational chemistry to computational medicinal chemistry: An open course on the	Yoshiro Nakata	Gunma University							C7
C32_153	Instability of network modules uncovers disease modules	Masataka Kikuchi	Tokyo Medical and Dental University						C6	
C33_156	Simulation of K+ ion flux in the gap junction network in cochlea in the inner ear	Eiichi Ueno	Tokyo Medical and Dental University						C6	
C34_23	Rapid detection of clinically important SNP 2269G>A in human ABCC4 gene using SmartAmp assay and its clinical validation	Wanping Aw	Tokyo Medical and Dental University	C1						
C35_158	Classification of steroid-binding proteins based on atomic environment and molecular function	Yasuha Tanaka	Tokyo Medical and Dental University				C4			
C36_167	Genome wide association study and pathway analysis (GWASPA) of atherosclerosis in three distinct arterial systems	Syed Ali Zaidi	Tokyo Medical and Dental University	C1						
C37_63	The bioluminescence-based odor sensing system with a yeast expressing an olfactory receptor	Yosuke Fukutani	Tokyo University of Agriculture and Technology			C3				
C38_66	Development of dehalococcoides enriched culture that grows on cis-1,2 dichloroethene and its metagenomic characterization by 2nd generation sequencer SOLiD	Ayane Takechi	Tokyo University of Agriculture and Technology	C1						
C39_131	Functions of two strictly conserved arginine residues in Fe-type nitrile hydratase from Rhodococcus erythropolis N771	Takayuki Aihara	Tokyo University of Agriculture and Technology				C4			
C40_52	A local relaxation of the secondary structure in human deacetylase SIRT2 induced by macrocyclic peptide binding	Yoshiaki Tanida	Fujitsu Laboratories Ltd.				C4			
C41_73	An ontological approach to modeling of interoperable abnormalities in medicine	Yuki Yamagata	Osaka University							C7

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C42_154	Demonstrated examples of the four-body corrected fragment molecular orbital calculations	Chiduru Watanabe	University of Tokyo					C5		
C43_163	Interaction analysis in implicit solvent with ionic effect using fragment molecular orbital method	Yoshio Okiyama	University of Tokyo					C5		
C44_56	Fragment screening for FLT3 inhibitors	Nae Saito	University of Tokyo			C3				
C45_82	Synthesis and SAR studies of PIM1 kinase inhibitors	Hirofumi Nakano	University of Tokyo		C2					
C46_64	Optimal lipophilicity of sulfonium p-toluenesulfonate as anti-allergic drug	Yukio Tada	University of Tokyo		C2					
C47_71	Influence of the membrane lipid composition on the conformational change of G-protein coupled receptor	Md. Iqbal Mahmood	Chiba University				C4			
C48_2	Molecular network of ChIP-seq-based vitamin D receptor target genes supports a protective role of vitamin D in development of multiple sclerosis	Jun-Ichi Satoh	Meiji Pharmaceutical University	C1						
C49_43	Developmental strategy of CAST (cancer stromal targeting) therapy using DDS (Drug delivery system) and Imaging technology	Masahiro Yasunaga	National Cancer Center Hospital East			C3				
C50_11	Enzyme kinetics and diseases	Kazumi Omata	National Center for Global Health and Medicine						C6	
C51_102	Identification of stage-specific gene expression signatures in response to retinoic acid during the neural differentiation of mouse embryonic stem	Hideko Sone	National Institute for Environmental Studies						C6	
C52_6	Chemical database mining for matched molecular pairs toward multi-ADMET optimization	Kenichi Mori	Astellas Pharma Inc.		C2					
C53_109	Clustering and QSAR approach by the KY-methods	Kohtaro Yuta	In Silico Data Ltd.		C2					
C54_36	A chemogenomics approach to predict binding activities of ligands to GPCRs based on the GPCRSARfari data in the ChEMBL database	Nobuyoshi Sugaya	PharmaDesign Inc.		C2					
C55_58	Predicting SCN1A-related epilepsy phenotypes based on the functional effect in SCN1A with the amino-acid substitution.	Shuichi Yoshida	Hamamatsu University School of Medicine						C6	
C56_47	Improved CDPG algorithm for effective interpretation of metabolic syndrome causing risk factor combinations	Shun Kawai	Nagoya University	C1						
C57_101	Enhanced screening and understanding of Hypolipidemic peptides assisted by informatics	Kei Kanie	Nagoya University			C3				
C58_117	Structural similarity search of molecules using the neighborhood fragment spectra	Hiroaki Kato	Toyohashi University of			C3				
C59_151	Finding peptide binding sites on a protein with a parallel n-ary search tree algorithm	Takuya Nakagawa	Toyohashi University of				C4			
C60_32	Prediction of drug-target interaction network using adverse event report systems	Masataka Takarabe	Kyoto University			C3				
C61_1	An approach to chemical education at medical technologist training institutions in Japan	Hidestugu Kohzaki	Kyoto University							C7
C62_5	Regulatory T cell-specific transcriptional regulation primed by epigenetic conversion and Foxp3 expression	Hiromasa Morikawa	Osaka university	C1						
C63_75	LigandBox : a database for 3D conformers of chemical compounds	Takeshi Kawabata	Osaka University						C6	
C64_55	On Swarm networks and molecular robots	Teijiro Isokawa	University of Hyogo						C6	

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C65_41	Optimization of PSMA-binding peptides by molecular modeling and binding energy prediction	Yasuyuki Fujii	Okayama University					C5		
C66_50	Large-scale quantum chemical calculations for the drug effects of AIDS agents	Yoichiro Yagi	Okayama University of Science					C5		
C67_26	A novel and consistent approach to enzymatic reactions using Ab initio MO calculations: Trypsin catalysis of a series of substrates	Akira Mashima	University of Tokushima					C5		
C68_27	A novel fragment based QSAR using FMO and LERE: binding affinity of relenza and its analogues with influenza virus neuraminidase	Hiroshi Matoba	University of Tokushima					C5		
C69_28	A new efficient approach to solvation energy change associated with complex formation of ligand with protein: critical comparison of various solvation energy calculations	Seiji Hitaoka	University of Tokushima					C5		
C70_24	A combined QM/MM (ONIOM) and QSAR approach to the study of complex formation of matrix metalloproteinase-9 with a series of biphenylsulfonamides	Tatsusada Yoshida	University of Tokushima					C5		
C71_134	searching multiple SNP associations in genome wide association study	Naoto Ikeda	Kyushu Institute of Technology	C1						
C72_65	Inferring chemogenomic features from drug-target interaction network using sparse canonical correspondence analysis	Yoshihiro Yamanishi	Kyushu University						C6	
C73_59	Identification of novel chemical inhibitors for hepatocyte growth factor by In silico structure-based drug screening	Yuji Koseki	Kyushu Institute of Technology			C3				
C74_99	Identification of novel small-molecule inhibitors of HIV-1 transcription by in silico screening	Takayuki Hamasaki	Kagoshima University			C3				
C75_4	Multi-parameter optimization in drug discovery: Quickly targeting compounds with a good balance of properties	Sumie Tajima	Hulinks Inc.							C6