ポスターセッション

討論時間　P2801～P2847　奇数番号：7/28 17:00～18:00　　偶数番号：7/28 18:00～19:00

P2801　Inventing *in silico* spot method (peptide tips for identify peptide epitope) by automatization of Autodock3.0

Taiki KOJIMA[1], Katsuyoshi SAKAGUCHI[2]
(Aichi Cancer Center, Department of Gastroenterogical Surgery[1] KLIMERS, Laboratory of Bioinformatics[2])

P2802　Drug-resistant Mechanism of Human Immunodeficiency Virus Type-1 Protease - Investigation by Molecular Dynamics Simulation -

Hirotaka OHDE[1], Masayuki HATA[1], Saburo NEYA[1], Wataru SUGIURA[2], Tyuji HOSHINO[1]
(Graduate School of Pharmaceutical Sciences, Chiba University[1], AIDS Research Center, National Institute of Infectious Diseases[2])

P2803　Modeling of Protein-Ligand Complexes Taking into Account the Induced Fit: Conformational and Positional Refinements Using Brownian Dynamics

Noriyuki YAMAOTSU[1], Ryuichi KAKURAI[1], Shuichi HIRONO[1]
(School of Pharmaceutical Sciences, Kitasato University[1])

P2804　FCANAL: a structure based protein function prediction method. Application to enzyme active sites and metal binding sites.

Ayumi SUZUKI[1], Tadashi ANDO[1], Satoru MIYAZAKI[2], Ichiro YAMATO[1]
(Department of Biological Science and Technology, Tokyo University of Science[1], Department of Pharmaceutical Sciences, Tokyo University of Science[2])

P2805　Sievgene: Protein-ligand flexible docking program based on grid potential and geometric hashing

Yoshifumi FUKUNISHI[1], Haruki NAKAMURA[1,2]
(Japan Biological Information Research Center (JBIRC), National Institute of Advanced Industrial Science and Technology (AIST)[1], Institute for Protein Research, Osaka University[3])

P2806　Computational Chemistry Analysis on the Interaction of Drugs and Water Molecules

Sumihiro HONJO[1], Hideyuki TSUBOI[2], Michihisa KOYAMA[1], Momoji KUBO[1,3], Kazumi NISHIJIMA[2,4], Tetsuya TERASAKI[2,5], and Akira MIYAMOTO[1,2]
(Dept. Appl. Chem., Tohoku Univ.[1], NICHe, Tohoku Univ.[2], JST-PRESTO[3], Mochida Pharmaceutical Co.[4], Dept. Pharm., Tohoku Univ.[5])

P2807 Computational Chemistry Apporach for the Prediction of Pharmacokinetics

Michihisa KOYAMA[1], Mohamed ISMAEL[1], Kosei SUGAWARA[1], Sumihiro HONJYOU[1], PEI Qiang[1], Hideyuki TSUBOI[2], Momoji KUBO[1,3], Kazumi NISHIJIMA[2,4], Tetsuya TERASAKI[2,5], Akira MIYAMOTO[2,1]

(Department of Applied Chemistry, Tohoku University[1], New Industry Creation Hatchery Center, Tohoku University[2], PRESTO, Japan Science and Technology Agency[3], Research & Development Division, Mochida Pharmaceutical Co. Ltd.[4], Graduate School of Pharmaceutical Sciences, Tohoku University[5])

P2808 Computational Chemical Study on Interactions among Lipid Bilayers, Proteins and Organic Drug Molecules

PEI Qiang[1], Hideyuki TSUBOI[2], Michihisa KOYAMA[1], Momoji KUBO[1,3], Kazumi NISHIJIMA[2,4], Tetsuya TERASAKI[2,5], Akira MIYAMOTO[1,5]

(Department of Applied Chemistry, Tohoku University[1], New Industry Creation Hatchery Center, Tohoku University[2], PRESTO, Japan Science and Technology Agency[3], Research & Development Division, Mochida Pharmaceutical Co. Ltd.[4], Graduate School of Pharmaceutical Sciences, Tohoku University[5])

P2809 Conformational changes of the NADPH oxidase p47phox-p22phox complex: A Computational Chemical Study

Yoko WATANABE[1], Hideyuki TSUBOI[2], Michihisa KOYAMA[1], Momoji KUBO[1,3], Eiichiro ICHIISHI[2], Masahiro KOHNO[2], Akira MIYAMOTO[1,2]

(Dept. Appl. Chem., Tohoku Univ.[1], NICHe, Tohoku Univ.[3], JST-PRESTO[2])

P2810 A Consensus Approach for Identifying the Stabilizing Residues in (a/b)8 Barrel Proteins

M. Michael GROMIHA[1,*], Gerard PUJADAS[2], Csaba MAGYAR[3], S. SELVARAJ[4] and Istvan SIMON[3]

([1]Computational Biology Research Center (CBRC), Institute of Advanced Industrial Science and Technology (AIST), 2-43 Aomi Koto-ku Tokyo 135-0064 Japan, [2]Departament de Bioquímica i Biotecnologia, Universitat Rovira i Virgili Spain, [3]Institute of Enzymology Biological Research Center Budapest Hungary, [4]Department of Physics Bharathidasan University Tiruchirapalli 620 024 India)

P2811 Development of A Cell-based Assay System for Screening Drug Candidates and Analyzing Gene Functions

Takako SAKAMOTO[1], Arinobu TOJO[2], Jun NAKAYA[1], Akira SASAKI[1], Hideki TANUMA[1], Shigetaka ASANO[2], Tetsuo SHIMIZU[1]
(Division of Medical Data Processing Network System[1] and Division of Molecular therapy[2], Advanced Clinical Research Center, The Institute of Medical Science, The University of Tokyo)

P2812 High-throughput estimation of the initial DNA concentration using real-time PCR

Osamu GOTO[1], Takashi NAKAJIMA[2], Akira SUYAMA[1]
(University of Tokyo[1], NovusGene Inc.[2])

P2813 Development of the Total System ‘ToMoCo’ for Molecular Design

Masamoto ARAKAWA[1], Soichiro MIZOBUCHI[2], Kimito FUNATSU[1]
(The University of Tokyo[1], Toyohashi University of Technology[2])

P2814 “BioSerendip” A Support System for Bio Researches

Akira IIDA, Hideya UEHARA, Kouichi OHKUBO, Junji FUKUMOTO
(SGI japan Ltd.)

P2815 An auto-modeling program of carbohydrate chains: its development and application to molecular dynamics simulations

Kenichi MORI, Masayuki HATA, Saburo NEYA, Tyuji HOSHINO
(Graduate School of Pharmaceutical Sciences, Chiba University, Department of Physical Chemistry)

P2816 Novel Mechanism of Site-specific Asparaginyl Racemization in Mouse Lysozyme

Keisuke UENO[1], Hideki TAKEHARA[2], Masahiro OKAMOTO[1]
(Kyushu Univ., Grad. Sch. Biores. Bioenv. Sci.[1], Fukuoka Int. Univ., Fac. Int. Commmun.[2])

P2817 De novo peptide sequencing used by amino acid binding affinity for tandem mass spectrometry

Mitsuhiro KANAZAWA[1], Atsushi OGIWARA[2], Unpei NAGASHIMA[1]
(Department of Chemistry, Graduate School of Pure and Applied Sciences, University of Tsukuba[1], Medical ProteoScope, Co. Ltd.[2])

P2818 Stochastic Simulation method for reaction-diffusion systems and its application to mitogen-activated protein kinase cascade pathway

Ryuzo AZUMA[1], Yoshiki YAMAGUCHI[1], Tomoyuki YAMAMOTO[2], Akihiko KONAGAYA[1]
(Genomic Sciences Center, RIKEN[1], School of Knowledge Science, JAIST[2])

P2819 A Data-mining system for discovering drug-target proteins

Motoi TOBITA, Masashi NEMOTO, Ken HORIUCHI, Hiroyasu SHIMADA, and Tetsuo NISHIKAWA
(Informatics department, Reverse Proteomics Research Institute Co. Ltd.)

P2820 Theoretical study of PPAR gamma mutations in type 2 diabetes mellitus

Narutoshi KAMIYA[1], Takuma SHIRAKI[2], Takashi S. KODAMA[3], Hisato JINGAMI[2]
(Department of Computational Biology[1], Molecular Biology[2], Structural Biology[3], Biomolecular Engineering Research Institute (BERI))

P2821 Assessment of somachlonal variation in *Arabidopsis thaliana* callus caused during subculture

Yoshinori MURATA, Takahito WATANABE[a)], Yuji FUKUDA, and Hitoshi IWAHASHI
(International Patent Organism Depositary, AIST, [a)]Research Institute for Sustainable Humanosphere (RISH), Kyoto University)

P2822 Sampling Methods on Microorganism Mutagenicity Prediction by Pattern Recognition

Kohtaro YUTA[1], Katsuhiko SAWATARI[2], Yoshifumi NAKANISHI[2], Taijiro MATSUSHIMA[3]
(Fujitsu Ltd.[1], National Institute of Industrial Health[2], Japan Bioassay Research Center[3])

P2823 The mathematical analysis of yeast Complex Complex Interactions

So NAKAGAWA, Yasuhiro SUZUKI, Soichi OGISHIMA, Takeshi HASE, Hiroshi TANAKA
(Graduate School of Tokyo Medical and Dental University)

P2824 Latest Developments in ProNIT (Thermodynamic Database for Protein-Nucleic Acid Interactions)

M. D. Shaji KUMAR[1], Ponraj PRABAKARAN[2], Hatsuho UEDAIRA[1], M. Michael GROMIHA[3], Kouji KITAJIMA[1] and Akinori SARAI[1]
(KIT, 680-4 Kawazu, Iizuka-shi, Fukuoka 820-8502[1], NIH, USA[2], CBRC, AIST, 2-41-6 Aomi, Koto-ku, Tokyo 135-0064[3])

P2825 Development and application of a molecular dynamics simulation system : prestoX

Yoshiaki MIKAMI[1], Yoshifumi FUKUNISHI[2], Ikuo FUKUDA[1], Jae Gil KIM[1], Yukihisa S WATANABE[1], Rie TATSUMI[1], Masaru HORIE[1], Haruki NAKAMURA[3]
(Japan Biological Information Research Center (JBIRC), Japan Biological Informatics Consortium (JBIC)[1], Biological Information Research Center (BIRC), National Institute of Advanced Industrial Science and Technology (AIST)[2], Institute for Protein Research, Osaka University[3])

P2826 Outcome prediction from gene expression based Support Vector Machine

Chihoko TAGO, Taizo HANAI, Masahiro OKAMOTO
(Laboratory for Bioinformatics, Graduate School of Systems Life Sciences, Kyushu University)

P2827 Identification of novel p53 target genes by the in-silico analysis

Reo MARUYAMA[1,4], Minoru TOYOTA[1,2], Hirofumi AKASHI[1,3], Fumio AOKI[3], Yasushi SASAKI[1,2], Hiroaki MITA[1,2], Hideki KAKIUCHI[4], Takashi TOKINO[2], Kohzoh IMAI[1]
(First Department of Internal Medicine[1], Department of Molecular Biology[2], Information Center of Computer Communication Sapporo Medical University[3], Jikeikai Hospital[4])

P2828 The structure–activity relationship of P-glycoprotein

Hiroyuki HIRANO[1], Yuko ONISHI[1,2], Toshihisa ISHIKAWA[2]
(GS platZ Co. Ltd.[1], Tokyo Institute of Technology[2])

P2829 The Unmasking of Putative Susceptivility Genes in Prostate Cancer Using Gene Expression Analysis

Uyen T. NGUYEN[1], Ilya KUPERSHMIDT[2], Barrett P. EYNON[3], Anoop GREWAL[4], Akio TANABE[5]
(Silicon Genetics[1])

P2830 Global gene expression profiles of pretreatment on freeze-thaw stress of yeast

Yuko MOMOSE[1], Hitoshi IWAHASHI[1]
(National Institute of Advanced Industrial Science and Technology (AIST)[1])

P2831 Screening of CRP-binding DNA sequence using mutation matrices derived from systematic single base-pair substitution experiments

Katsumi OMAGARI[1], Hidehisa YOSHIMURA[2], Mitunori TAKANO[3], Masayuki OHMORI[2,4], Akinori SARAI[5], Akira SUYMA[1]
(Univ. of Tokyo[1], Toho Univ.[2], Waseda Univ.[3], Saitama Univ.[4], Kyushu Inst. Tech.[5])

P2832 Molecular Docking of the Compounds Activate Like Ecdysis Hormone with its Receptor

Tadayoshi FUKUDA, Shinji TANIMORI, Mitsunori KIRIHATA
(Department of Applied Biochemistry, Osaka Prefecture University)

P2833 Reconstructing Longitudinal Phylogenetic Tree of HIV-1 Protease Gene by inking Within-patient Orthologous Viral Population under HAART

Naoki HASEGAWA[1], Wataru SUGIURA[2], Fengrong REN[1], Zene MATSUDA[2], Hiroshi TANAKA[1]
([1]Department of Bioinfomatics, Biomedical Science PhD Program, Tokyo Medical and Dental University. Tokyo, Japan. [2]AIDS Research Center, National Institute of Infectious Diseases, Tokyo, Japan)

P2834 Multiple Docking with Target Protein: A Novel Drug Design Strategy with Xsi

Kazuto YAMAZAKI[1], Masaharu KANAOKA[1], Yuichiro INAGAKI[2]
(Sumitomo Pharmaceuticals Co. Ltd.[1], Fuji Research Institute Corporation[2])

P2835 Structural analyses of metabolic networks using GNU Octave

Jun OHTA[1]
(Okayama University Graduate School of Medicine and Dentistry[1])

P2836 *High-Speed Screening and Structure-Activity Relationship Analysis* for the Evaluation of Drug-Drug Interactions of Human ABCG2 (BCRP)

Toshihisa ISHIKAWA[1], Hikaru SAITO[1], Yuko ONISHI[1], Keisuke OOSUMI[2], Takaaki FUKAMI[2], Makoto NAGAKURA[2], Shigeru TARUI[3], and Hiroyuki HIRANO[3]
(Tokyo Institute of Technology[1], BioTec Co. Ltd.[2], GS PlatZ Co. Ltd.[3])

P2837 *In silico* Discovery of the Peroxisomal Proteome

Igor V. KUROCHKIN[1], Takeshi NAGASHIMA[1], Akihiko KONAGAYA[2] and Christian SCHÖNBACH[1]
([1]Immunoinformatics Team, [2]Bioinformatics Group, RIKEN Genomic Sciences Center, Yokohama, Japan)

P2838 SPR assays for lead optimization in drug discovery

Robert KARLSSON[1], Helena WIDEGREN[1], Helena NORDIN[1], Annie NASLUND[1] and Asa Frostell KARLSSON[1], Issey OKAZAKI[2], Setsuko HASHIMOTO[2]
(Biacore AB[1](Sweden), Biacore K.K.[2])

P2839 Gene network analysis of mRNA expression pattern with interferon efficacy to hepatitis C patient.

Akito DAIBA[1,3], Kazuhiro HAYASHIDA[2], Takako FURUYA[1], Satoru ITOU[1], Masafumi YOHDA[3]
(Japan Genome Solutions[1], Sasebo Kyosai Hospital[2], Tokyo University of Agriculture and Technology[3])

P2840 Validation and Improvement of Charge Equilibration Methods with Empirical Two-Center Coulombic Terms

Akifumi ODA[1], Shuichi HIRONO[2]
(Toyama chemical Co. Ltd.[1], School of Pharmaceutical Sciences, Kitasato University[2])

P2841 Conformation Estimation of Collagen Derived Oligopeptides by Tsallis Entropy adopted Simulated Annealing

Hisaki NAKABAYASHI, Yuuichi TOKUDA, Koichi TAKAHASHI
(Graduate School of Science and Technology, Kinki University)

P2842 Genome wide annotation of Thermus thermophilus HB8

Akinobu FUKUZAKI[1,2], Takeshi NAGASHIMA[1], Kaori IDE[1,2], Fumikazu KONISHI[1,2], Mariko HATAKEYAMA[1,2], Shigeyuki YOKOYAMA[2,3,4], Seiki KURAMITSU[2,5] and Akihiko KONAGAYA[1,2]
([1]Bioinformatics G., RIKEN, GSC, [2]RIKEN Harima Inst., [3]Protein Res. G., RIKEN GSC, [4]Grad. Sch. Of Sci., Univ. of Tokyo. [5]Grad. Sch. Of Sci., Osaka Univ.)

P2843 Development of a novel bioinformatics approach to selecting mucin-like proteins

Chikako NISHI-TAKAOKA[1,2], Takahiro SHIMAMURA[1], Shogo YAMAMOTO[1], Yoshitaka HIPPO[1], Tatsunari NISHI[1], and Hiroyuki ABURATANI[1]
(RCAST, The Univ. of Tokyo[1], Ochanomizu Univ.[2])

P2844 A Theoretical Study on Octanal Recognition of the Olfactory Receptor Protein ORI7

Junko TAGUCHI[1,2], Sachiko AIDA-HYUGAJI[3], Kaori UENO-NOTO[1], Fumiko YOSHII[1], Keiko TAKANO[1]
(Ochanomizu University[1], TAIHO Pharmaceutical Co. Ltd.[2], Tokai University[3])

P2845 A system evaluation of site scalability and throughput performance of homology search tool on grid

Fumikazu KONISHI[1], Akihiko KONAGAYA[1]
(Bioinformatics Group, RIKEN Genomic Sciences Center[1])

P2846 Analysis of the interaction of mannotriose with anti-HIV protein, Actinohivin

Masahide KUROSAKI[1], Noriyuki YAMAOTSU[1], Atsushi TAKAHASHI[1], Junji INOKOSHI[1], Haruo TANAKA[1], Satoshi OMURA[2], Shuichi HIRONO[1]
(School of Pharmaceutical Sciences, Kitasato University[1], Kitasato Institute for Life Sciences, Kitasato University[2])

P2847 Construction of Knowledge Library for analysis of microarray data in Arabidopsis thaliana

Yoshikazu HASEGAWA[1], Motoaki SEKI[2], Masakazu SATOU[1], Tetsuya SAKURAI[1], Kenji AKIYAMA[1], Kei IIDA[3], Naoki OKAMOTO[4], Katsura HIROSAWA[1], Tetsuro TOYODA[1], Kazuo SHINOZAKI[2], and Akihiko KONAGAYA[5]
(Genomic Knowledge Base Research Team, GSC, RIKEN[1], Plant Mutation Exploration Team, GSC, RIKEN[2], Faculty of Bio-Science, Nagahama Institute of Bio-Science and Technology[3], NEC Infomatec Systems Ltd.[4], Bioinformatics Group, GSC, RIKEN[5])

討論時間　P2901～P2948　奇数番号：7/29 17:00～18:00　　偶数番号：7/29 18:00～19:00

P2901 Classification of kinases using neural networks and physicochemical parameters of amino acids

Tomoko NIWA
(Discovery Research Laboratories, Nippon Shinyaku Co. Ltd., t.niwa@po.nippon-shinyaku.co.jp)

P2902 Infrastructure Model for Protocol Management Support in Translational Research

Akira SASAKI, Jun NAKAYA, Tetsuo SHIMIZU
(Institute of Medical Science, University of Tokyo)

P2903 STUDY ON A BINDING AFFINITY DIFFERENCE BETWEEN CHITINASE-ARGADIN AND CHITINASE-ARGIFIN COMPLEXES USING MOLECULAR DYNAMICS SIMULATION

Yuichi YANAI[1], Hiroaki GOUDA[1], Shuichi HIRONO[1]
(School of Pharmaceutical Sciences, Kitasato University[1])

P2904 The ionic status of TPI in the active thymidine phosphorylase state

Yukio TADA[1],Makoto NOMURA[1], Shingo YANO[1], Hideki KAZUNO[1], Tutomu SATO[1], Masakazu FUKUSHIMA[1], Tetsuji ASAO[1]
(Hanno Research Center, Taiho Pharmaceutical Co. Ltd.[1])

P2905 Relations between self interaction proteins and evolutional conservation of densely connected topologies in the protein-protein interaction network.

Takeshi HASE[1], Soichi OGISHIMA[1], Yasuhiro SUZUKI[1,2], So NAKAGAWA[2], Hiroshi TANAKA[1,2]
(Dept. of Bioinformatics Tokyo Medical and Dental University[1], Dept. of Computational Biology Graduate School of Tokyo Medical and Dental University[2])

P2906 Molecular Dynamics Simulations of liganded and unliganded proteins

Noriaki OKIMOTO[1], Takashi NAKAMURA[2], Atsushi SUENAGA[1], Noriyuki FUTATSUGI[1], Yoshinori HIRANO[3], Makoto TAIJI[1], Akihiko KONAGAYA[1], Isamu YAMAGUCHI[2], and Toshikazu EBISUZAKI[3]
(RIKEN, GSC[1], RIKEN Plant Science Center[2], RIKEN Wako[3])

P2907 Computational Chemistry Study on Theophylline Metabolism with Different Tissues Components

Mohamed ISMAEL[1], Hideyuki TSUBOI[2], Michihisa KOYAMA[1], Momoji KUBO[1,3], Kazumi NISHIJIMA[2,4], Tetsuya TERASAKI[2,5], Akira MIYAMOTO[1,2]
(Department of Applied Chemistry, Tohoku University[1], New Industry Creation Hatchery Center, Tohoku University[2], JST-PRESTO[3], Research & Development Division, Mochida Pharmaceutical Co. Ltd.[4], Graduate school of Pharmaceutical Sciences, Tohoku University[5])

P2908 Development of a simulation and analysis support system for molecule science

Takashi IKEDA[1], Susumu HANDA[1], Atsushi SENGOKU[1], Eiju KANAZAWA[2], Toshihiro SAKUMA[1], Toshikazu TAKADA[3]
(NEC Infomatec system Ltd.[1], Navie[2], NEC Copporation[3])

P2909 BioStation Dock: Application of protein-ligand docking to screen compounds (2)

Toshiyuki SATO[1], Kaori FUKUZAWA[1], Kozo AOKI[3], Katsuki AMEMIYA[2], Kazuo KOYANO[2], Shinji AMARI[3], Souichirou TANIMORI[2], and Tatsuya NAKANO[4]
(Fuji Research Institute Corporation[1], AdvanceSoft Corporation[2], University of Tokyo[3], and National Institute of Health Sciences[4])

P2910 *In Silico* screening for Nuclear Receptor Target Genes

Yoshitomo TANAKA[1], Tsuguchika KAMINUMA[2], Kotoko NAKATA[3], Hiroshi TANAKA[4]
(Graduate school of Tokyo Medical and Dental University[1], Biodynamics Inc.[2], National Institute of Health Sciences[3], Medical Research Institute, Tokyo Medical and Dental University[4])

P2911 Generation of novel equations for logP, solubility, pKa using a neural network

Kenji YAMAGISHI[1], Sumie TAJIMA[2], Toru YAGI[2], Makoto HARAGUCHI[2], Hiroaki TOKIWA[1], Umpei NAGASHIMA[3]
(Rikkyo University[1], Bestsystems INC.[2], National Institute of Advanced Industrial Science and Technology[3])

P2913 E-pathfinder

Sayaka KAGEKAWA[1], Jun NAKAYA[2], Tetsuo SHIMIZU[2]
(Fujitsu Advanced Solutions LTD.[1], Institute of Medical Science of the University of Tokyo[2])

P2914 Structural Analysis of the Binding Sites in the Protein-Protein Interaction

Tsuyoshi HAMADA, Kaori FUKUZAWA, Toshiyuki SATO
(Fuji Research Institute Corporation)

P2915 Molecular dynamics simulation of reaction mechanism of Estrogen Receptor

Yoshiro NAKATA and Yoko KANAZAWA
(Department of Biophysics, Faculty of Engineering, Gunma University)

P2916 Investigation of species specificity in ligand-dependent PPARa activation using molecular modeling approach

Hideharu UCHIKI
(Discovery Research Laboratories, Kyorin Pharmaceutical Co. Ltd.)

P2917 Development of Pharmacokinetic Simulator based on Three-Dimensional Graphics

Kotaro OKUSHI[1], Hideyuki TSUBOI[1], Michihisa KOYAMA[1], Momoji KUBO[1,3], Kazumi NISHIJIMA[2,4], Tetsuya TERASAKI[2,5], Akira MIYAMOTO[1,4]
(Department of Applied Chemistry, Tohoku University[1], New Industry Creation Hatchery Center, Tohoku University[2], PRESTO, Japan Science and Technology Agency[3], Research & Development Division, Mochida Pharmaceutical Co. Ltd.[4], Graduate School of Pharmaceutical Sciences, Tohoku University[5])

P2918 In silico screening for endogenous surrogate compounds interacting with a GPCR

Takeshi HIRAMOTO[1], Yosuke NONAKA[1], Kazuko INOUE[1], Mariko OMATSU-KANBE[2], Hiroshi MATSUURA[2], Keigo GOHDA[3], and Norihisa FUJITA[1]
([1]Ritsumeikan University, [2]Shiga University of Medical Science, [3]CAMM-Kansai)

P2920 Biomarker detection and disease classification alogorithm using SELDI-TOF-MS

Kaoru MOGUSHI[1], Fumio NOMURA[2], Hiroshi TANAKA[1]
(Department of Bioinformatics, Tokyo Medical and Dental University[1], Department of Molecular Diagnosis, Chiba University[2])

P2921 Feature extraction of gene expression onset time for cluster analysis

Kazumi HAKAMADA[1], Taizo HANAI[1], Masahiro OKAMOTO[1]
(Laboratory for Bioinformatics, Graduate School of Systems Life Science, Kyushu University[1])

P2923 Microarray Data Analysis Using Fuzzy K-means Clustering

Chinatsu ARIMA, Taizo HANAI, Masahiro OKAMOTO
(Laboratory for Bioinformatics, Graduate School of Systems Life Sciences, Kyushu University)

P2924 Structural analysis by molecular dynamics simulations: Protein-protein interactions of Ras-Raf and Ras-RalGDS complexes

Noriyuki FUTATSUGI[1], Mikako SHIROUZU[2], Atsushi SUENAGA[1], Noriaki OKIMOTO[1], Tetsu NARUMI[1], Toshikazu EBISUZAKI[3], Shigeyuki YOKOYAMA[2], Makoto TAIJI[1], Akihiko KONAGAYA[1]
(Bioinformatics Group, RIKEN Genomic Sciences Center[1], Protein Research Group, RIKEN Genomic Sciences Center[2], Ebisuzaki Computational Astrophysics Laboratory, RIKEN[3])

P2925 Profiling of Genome-wide expression under hydrostatic pressure stress in the yeast Saccharomyces cerevisiae

Hisayo SHIMIZU, Hitoshi IWAHASHI
(National Institute of Advanced Industrial Science and Technology International Patent Organism Depositary)

P2926 QSAR Analysis of Human Placental Drug Transport

Yuki HIBINO, Takashi FUJIWARA, Shinichi KOBAYASHI, Kumiko SAKAMOTO, Masaru KIHARA, Aiko YAMAUCHI, Hiroshi CHUMAN
(Graduate School of Pharmaceutical Sciences, The University of Tokushima)

P2927 Microarray cluster analysis of *Saccharomyces cerevisiae* gene expression under different chemicals stress conditions

Yoshiteru SUZUKI, KIM Hyun-Ju, Yuko MOMOSE, Hitoshi IWAHASHI
(National Institute of Advanced Industrial Science and Technology (AIST))

P2928 Janus-type Go model: toward a theory for the kinetic control of protein functions

Hironori K. NAKAMURA[1,2], Mitsunori TAKANO[1]
(Dept. of Phys., Sch. of Sci. & Eng., Waseda Univ.[1], ACT-JST, JST[2])

P2929 Construction of the XML Database of the Pharmaceutical Reference

Masaki HAMADA, Shinya TAKIGUCHI, Mamoru HIROTA, Kaori KURATA, Akira DOBASHI
(Tokyo University of Pharmacy and Life Science)

P2930 Xsi – An integrated system for drug discovery

Yuichiro INAGAKI[1], Michiaki HAMADA[1], Kazuto YAMAZAKI[2], Masaharu KANAOKA[2], Hiroshi CHUMAN[3]
(Fuji Research Institute Corporation[1], Sumitomo Pharmaceuticals Co. Ltd.[2], Tokushima

P2931 Reaction mechanism of biodegradable plastics degrading enzyme

Yoshitake SAKAE[1], Misako AIDA[1], Hidemasa KONDOU[2], Kazuo MASAKI[3], Haruyuki IEFUJI[3]
(Hiroshima University-Center for Quantum Life Sciences[1], National Institute of Advanced Industrial Science and Technology[2], National Research Institute of Brewing[3])

P2932 A New Approach to Drug Molecular Design based on Neural Network Analysis and Molecular Orbital Calculation : Molecular Modeling to Circumvent Cancer Drug Resistance Associated with ABCG2

Sachiko AIDA-HYUGAJI[1], Jumma NOMURA[2], Minoru SAKURAI[2], Daisuke TOKUSHIMA[3], Toshikazu TAKADA[3], Umpei NAGASHIMA[4] and Toshihisa ISHIKAWA[2]
(Tokai University[1], Tokyo Institute of Technology[2], NEC Corporation[3], National Institute of Advanced Industrial Science and Technology[4])

P2933 Implementation of MP2-correlation engine into ABINIT-MP/FMO program and emonstrative applications

Yuji MOCHIZUKI[1,2], Tatsuya NAKANO[3] , Shigeru KOIKEGAMI[2] , Shinji AMARI[1], Kazuo KITAURA[4]
(Institute for Industrial Science, The University of Tokyo[1], Advancesoft[2], National Institute of Health Science[3], National Institute for Advanced Industrial Science and Technology[4])

P2934 Computer-aided rational molecular design of a new chitinase inhibitor

Hiroaki GOUDA[1], Yusuke SAKOH[1], Shuichi HIRONO[1]
(School of Pharmaceutical Sciences, Kitasato University)

P2935 FREP: a system for inferring of functional repeats

Takeshi NAGASHIMA[1], Christian SCHÖNBACH[1], Igor V. KUROCHKIN[1], Akihiko KONAGAYA[2]
([1]Immunoinformatics Team, [2]Bioinformatics Group, RIKEN Genomic Sciences Center, Yokohama, Japan)

P2936 SOLUTION STRUCTURE OF HUMAN SERUM ALBUMIN OBTAINED FROM MOLECULAR DYNAMICS SIMULATION

Taku FUJIMOTO, Yasuo MATSUSHITA, Hiroaki GOUDA, Shuichi HIRONO
(School of Pharmaceutical Sciences, Kitasato University)

P2937 Development of a potal for drug discovery

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P2938 MOLDA QuLiS: Development of Molecular Modeling Program for Structure-based Drug Design

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P2939 Catalytic Roles of Active-Site Amino Acid Residues of Coenzyme B_{12}-Dependent Diol Dehydratase: A Quantum Mechanical/Molecular Mechanical (QM/MM) Study

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P2940 Theoretical study of methane hydroxylation by methane monooxygenase

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P2941 QM/MM Study of the Mononuclear Non-heme Iron Active Site of Phenylalanine Hydroxylase

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P2942 Novel screening method for functional nucleotide and its motif extraction

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P2943 Analysis of Ternary Structures Constructed by Protein Modeling Tool, PDFAMS Pro+

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P2944 Molecular Recognition System in Pheromone-Pheromone Binding Protein Complex Analyzed by FMO method: Structure Optimization of Ligand and Its Binding Pocket.

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P2945 Drug Target Database based on Therapeutic Classification

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P2947 HIGH-THROUGHPUT SCREENING SYSTEM OF PROTEIN CRYSTALLIZATION CONDITIONS USING MICROFLUIDIC REACTOR ARRAY

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P2948 Toward an Automatic Extraction of the Drug Interaction-related Expressions

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