ポスターセッション

討論時間　奇数番号：9/18　17:00-18:00　偶数番号：9/18　18:00-19:00

1. 分子計算

101 Computational Chemistry Investigation of Water Interface in Colloidal Systems

Ugur Mart[1], Ryuji Miura[1], Chang-ho Jung[1], Takahiro Oyama[1], Akira Endou [1], Momoji Kubo [1], Akira Miyamoto [1,2]

(Dept. of Appl. Chem., Tohoku Univ.[1], NICHe, Tohoku Univ.[2])

102 Effect of organic moieties on the acidic properties of zeolite with an organic lattice as a new candidate for drug synthesis

Mohamed Elanany[1], Akira Endou[1], Momoji Kubo[1] and Akira Miyamoto[1,2]

([1]Department of Applied Chemistry, Graduate School of Engineering, Tohoku University, [2]New Industry Creation Hatchery Center, Tohoku University)

103 Theoretical Investigation of Excited State and Excitation Processes for Several Compounds

Xiaojing Wang[1], Lv Chen[1], Akira Endou[1], Momoji Kubo[1], Akira Miyamoto[1,2]

(Dept. Appl. Chem. Tohoku Univ.[1], NICHE Tohoku Univ.[2])

104 Computational Study on the Conformation of the Complex of Lipase Enzyme with Foreign Organic Substrate

Yoshinobu Naoshima[1], Yoshihiro Mori[2], Takatomo Kimura[3], Makoto Kamezawa[3], Hojun Tachibana[3], and Takehiko Ohtani[3]

(Okayama University of Science[1], Graduate School of Okayama University[2], and Konan Chemical Industry Co., Ltd.[3])

105 Protein-ligand flexible docking method for *in silico* screening

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 [2])

106 Molecular dynamics simulation of reaction mechanism of the hyperthermophilic aspartate racemase

Tomohiro Seko[1], Lijun Liu[2], Takumitsu Yoshida[3], Kunio Miki[2], Masafumi Yohda[3]

(Fuji Xerox Co., Ltd.[1], Graduate School of Science, Kyoto University[2], Faculty of Engineering, Tokyo University of Agriculture and Technology[3])

107 Harmonic Force Field Parameterization based on Hessian matrix

Hirotaka Ohde[1], Daisuke Katagiri[1], Hidenori Ishikawa[1], Saburou Neya[1], Masayuki Hata[1], Tyuji Hoshino[1]

(Graduate School of Pharmaceutical Sciences, Chiba University[1])

108 Development of a molecular dynamics simulation system : prestoX

Yoshiaki Mikami[1,2], Yoshifumi Fukunishi[1], Ikuo Fukuda[1,2], Jae Gil Kim[1,2], Rie Tatsumi[1,2], Haruki Nakamura[1,3]
(Biological Information Research Center (BIRC), National Institute of Advanced Industrial Science and Technology (AIST) [1], Japan Biological Information Research Center (JBIRC), Japan Biological Informatics Consortium (JBIC) [2], Institute for Protein Research, Osaka University [3])

109 Parallelization of Biomolecular Simulations through Replica Exchange Molecular Dynamics

Masakatsu Ito[1,2], Umpei Nagashima[1,2]
([1]Research and Development for Applying Advanced Computational Science and Technology of Japan Science and Technology Corporation, [2]Grid Technology Research Center, National Institute of Advanced Industrial Science and Technology (AIST))

110 Interaction analysis for SARS virus proteinase and its ligands with ab initio FMO method

Shinji Amari[1], Mayuko Takeda-Shitaka[2], Mitsuo Iwadate[2], Norio Yamamoto[3], Nobutaka Fujii[4], Naoki Yamamoto[3], Hideaki Umeyama[2], Tatsuya Nakano[5]
(University of Tokyo[1], Kitasato University[2], Tokyo Medical and Dental University[3], Kyoto University[4], National Institute of Health Sciences[5])

111 BioStation Dock: Application of protein-ligand docking to screen compounds

Toshiyuki Sato[1,2], Ikuo Okouchi[1,2], Kaori Fukuzawa[1,2], Kozo Aoki[3], Kazuo Koyano[1], Shinji Amari[3], Katsuki Amemiya[1], and Tatsuya Nakano[4]
(AdvanceSoft Corporation [1], Fuji Research Institute Corporation[2], University of Tokyo[3], and National Institute of Health Sciences [4])

112 Periodical Boundary Computational Chemistry Studies on Tribology Chemistry Reaction

Hui. Zhou[1], Akira Endou[1], Momoji Kubo[1], Akira Imamura[2], Akira Miyamoto[1,3]
(Graduate School of Engineering, Tohoku Univ.[1], Faculty of engineering, Hiroshima Kokusai Gukuin Univ.[2], New Industry Creation Hatchery Center, Tohoku Univ.[3])

113 Study on Photocatalytic Processes by Accelerated Quantum Chemical Molecular Dynamics Method

Chen Lv[1], Xiaojing Wang[1], Tomonori Kusagaya[1], Akira Endou [1], Momoji Kubo[1], Akira Imamura[2], and Akira Miyamoto[1,3]
(Department of Applied Chemistry, Tohoku University[1], Faculty of Engineering, Hiroshima Kokusai Gakuin University[2], NICHe, Tohoku University[3])

114 Accelerated quantum chemical molecular dynamics simulation and DFT studies on the catalytic reaction of lanthanocene

Yi Luo[1], Yuki Ito[1], Hitoshi Kurokawa[1], Akira Endou[1], Momoji Kubo[1], Akira Imamura[2], and Akira Miyamoto[1,3]

(Department of Applied Chemistry, Tohoku University[1], Faculty of Engineering, Hiroshima Kokusai Gakuin University[2], NICHe, Tohoku University[3])

115 Dynamic Observation of Nucleic Acid Structure by Molecular Dynamics

Satoshi Fujii, Takahiko Nojima and Shigeori Takenaka

(Department of Applied Chemistry, Faculty of Engineering, Kyushu University)

116 Accelerated Quantum Chemical Molecular Dynamics Study on the Unsaturated Hydrocarbon Polymerization

Huifeng Zhong[1], Masaki Fushimi[2], Akira Endou[1], Momoji Kubo[1], Akira Imamura[3], and Akira Miyamoto[1,4]

(Dept. Appl. Chem., Tohoku Univ[1]. Oita Research Center, R&D Department, SunAllomer Ltd[2]. Fac. Eng., Hiroshima Kokusai Gakuin Univ[3]. NICHe, Tohoku Univ[4].)

117 MD simulation of asymmetric phospholipid bilayers (POPC/POPE-POPS) with the physiological concentration of ions and cholesterols

Kenichi Mori, Masayuki Hata, Saburo Neya, Tyuji Hoshino

(Graduate School of Pharmaceutical Sciences, Chiba University)

118 Biosystem Modeling from Micro-Scale to Macro-Scale

Momoji Kubo [1], Kotaro Ohkushi [1], Yasuyuki Suzuki [1], Akira Endou [1], Kazumi Nishijima [2,3], Eiichiro Ichiishi [3], Masahiro Kohno [3], and Akira Miyamoto [1,3]

(Department of Applied Chemistry, Tohoku University [1], Pharmaceutical Consortium for Protein Structure Analysis [2], NICHe, Tohoku University [3])

119 Development of accelerated quantum molecular dynamics program "Colors" into lanthanide compounds

Yuki Ito[1], Chang-ho Jung[1], Yi Luo[1], Akira Endou[1], Momoji Kubo[1], Akira Imamura[2], Akira Miyamoto[3]

(Dept. Appl. Chem., Tohoku University[1], Hiroshima Kokusai Gakuin University[2], NICHe, Tohoku University[3])

120 Development of Kinetic Monte Carlo Simulator and Its Application to Analysis of Mass Transfer and Diffusion Phenomenon

Akira Endou[1], Hitoshi Kurokawa[1], Ryuji Miura[1], Momoji Kubo[1], and Akira Miyamoto[1, 2]

(Grad. School of Eng., Tohoku Univ.[1], NICHe, Tohoku Univ.[2])

121 Prediction of the Lubricous Characteristic by Computational Chemistry

Yohei Toyoda[1], Daisuke Kamei[1], Akira Endou[1], Momoji Kubo[1], Akira Miyamoto[1,2]

(Dept. Appl. Chem., Tohoku Univ. [1], NICHe, Tohoku Univ. [2])

122 Development of Quantum Chemical Simulation System for Proteins, ProteinDF

Fumitoshi Sato[1], Naoki Ihara[1], Tetsuya Ueno[1], Hiroyuki Otsuki[1], Tomoyuki Kinjo[1], Saisei Tahara[1], Naoki Tsunekawa[1], Yasuyuki Nishimura[1], Hajime Muta[1], Tamotsu Yoshihiro[1], Chong Hwang Lean[1], Yoshitaka Nishikawa[3], Sinya Muramatsu[3], Kazutoshi Okada[3], Toru Inaba[2], So Koike[2], Yasuo Nagamine[2], Hideaki Koike[2], Hiroshi Kashiwagi[1,2]
(Institute of Industrial Science, University of Tokyo[1], AdvanceSoft Corporation[2], Fuji Research Institute Corporation[3])

123 Theoretical Studies of Binding of Mannose-binding Protein to Monosaccharides

Sachiko Aida-Hyugaji[1,2], Keiko Takano[2], Toshikazu Takada[3], Haruo Hosoya[2], Naoya Kojima[1], Tsuguo Mizuochi[1], and Yasushi Inoue[1]
(Tokai University[1], Ochanomizu University[2], NEC[3])

124 The Simulation of Helix-Coil Transition by MD Caluculations

Yoshiro Nakata, Masami Uno
(Department of Biophysics, Faculty of Engineering, Gunma University)

125 Development of a Geometry Optimization Program for Proteins Based on ProteinDF System

Tomoyuki Kinjo[1], Naoki Ihara[1], Naoki Tsunekawa[1], Kazutoshi Okada[2], Nobutaka Nishikawa[2], Tetsuya Ueno[1], Fumitoshi Sato[1], Hiroshi Kashiwagi[1,3]
(Institute of Industrial Science, University of Tokyo[1], Fuji Research Institute Corporation[2], Advance Soft[3])

126 Temperature dependent kinetics and mechanism of the protein folding in a coarse-grained model using the native structure information

Hironori K. Nakamura[1,2], Mitsunori Takano[1]
(Dept. of Life Sci., Grad. Sch. of Arts & Sci., Univ. of Tokyo[1], ACT-JST, JST[2])

127 Fragment molecular orbital study for the interaction between cAMP receptor protein and DNA

Kaori Fukuzawa[1], Yuto Komeiji[2], Yasuo Sengoku[3], Katsumi Omagari[4], Mitsuo Takano[4], Akira Suyama[4], Shigenori Tanaka[5], and Tatsuya Nakano[6]
(Fuji Research Institute Corporation[1], National Institute of Advanced Industrial Science and Technology[2], Toyohashi University of Technology[3], The University of Tokyo[4], Toshiba Corporation[5], National Institute of Health Sciences[6])

128 A Theoretical Study on Proton Transport

Kazunori Bada[1], Yusuke Makino[1], Hitoshi Kurokawa[1], Akira Endou[1], Momoji Kubo[1], and Akira Miyamoto[1,2]
(Department of Applied Chemistry, Graduate School of Engineering, Tohoku University[1], New Industry Creation Hatchery Center, Tohoku University[2])

129 Molecular dynamics of C30 region in α-Lactalbumin

Yuji Kitai[1], Masashi Sonoyama[2], Yoichi Hagiwara[1], Matsuaki Terada[1], Kenta Nakai[3], Shigeki Mitaku[2]

(Tokyo University of Agriculture and Techcology[1], Nagoya University[2], The Institute of Medical Science, The University of Tokyo[3])

130 Application of Fragment Molecular Orbital Method to Calculations on Proteins with Zinc Atom

Takanori Harada[1], Tatsuya Nakano[2], Hiroaki Tokiwa[1]

(Rikkyo University[1], National Institute of Health Sciences[2])

131 Development of New Kinetic Monte Carlo Simulator for Ion Transport

Hitoshi Kurokawa[1], Kazunori Bada[1], Yusuke Makino[1], Akira Endou[1], Momoji Kubo[1], and Akira Miyamoto[1, 2]

(Department of Applied Chemistry, Graduate School of Engineering, Tohoku University[1], New Industry Creation Hatchery Center, Tohoku University[2])

132 Computational Chemistry Study of Metal Complexes: Structures and Reaction Dynamics

Rado RAHARINTSALAMA[1], Hiroaki MUNAKATA[2], Akira ENDOU[2], Momoji KUBO[2] Akira MIYAMOTO[1,2]

(Dept. of Appl. Chem., Tohoku Univ.[1], NICHe, Tohoku Univ.[2])

133 Accelerated quantum chemical molecular dynamics study on electronic properties of platinum cluster in water environment

Changho Jung[1], Akira Endou[1], Momoji Kubo[1], Akira Imamura[2] and Akira Miyamoto[1,3]

(Department of Applied Chemistry, Tohoku University[1], Hiroshima Kokusai Gakuin University[2], New Industry Creation Hatchery Center (NICHe)[3])

134 On the collective motion of macromolecules

Takashi Nakamura

(College of Industrial Technology, Nihon University)

135 Atomic Structures and Electronic States of Water Clusters: A Computational Chemistry Study

Yoko Watanabe[1], Daisuke Kamei[1], Takahiro Oyama[1], Ryuji Miura[1], Akira Endou[1], Momoji Kubo[1], Tomohiro Ogawa[2], Akira Miyamoto[1, 3]

(Dept. Appl. Chem., Tohoku Univ.[1], Tokyo Electric Power Company[2], NICHe, Tohoku Univ.[3])

136 Large Scale Quantum Chemical Molecular Dynamics of Surface Reaction with Ion Implantation

Katsumi Sasata[1], Akira Endou[1], Momoji Kubo[1], Akira Imamura[2], Akira Miyamoto[1,3]

(Tohoku Univ.[1], Hiroshima Kokusai Gakuin Univ.[2], NICHe, Tohoku Univ.[3])

137 Application of Accelerated Quantum Molecular Dynamics Method to the Investigation on the Electrode / Organic Molecules Interface

Yuhsuke Makino[1], Ken Suzuki[1], Akira Endou[1], Momoji Kubo[1], Akira Imamura[2], and Akira Miyamoto[1, 3]
(Grad. School of Eng., Tohoku Univ.[1], Dept. Eng., Hiroshima Kokusai Gakuin Univ.[2], NICHe, Tohoku Univ.[3])

138 Conformational Change of Calmodulin by Ca^{2+} and Peptide Removal

Li Hongzhen[1], Kiyonobu Yokota[2], Kenji Satou[1,2]
(Institute for Bioinformatics Research and Development (BIRD), Japan Science and Technology Corporation (JST)[1], School of Knowledge Science, Japan Advanced Institute of Science and Technology[2])

139 Computational Chemistry Study for Nanoscale Tribology

Takahiro Oyama [1], Akira Endou[1], Momoji Kubo[1], Akira Miyamoto[1,2]
(Dept. of Appl. Chem., Tohoku Univ.[1], NICHe, Tohoku Univ.[2])

2. 創薬テクノロジー

201 SOLUTION STRUCTURE OF CHITINASE-ARGIFIN COMPLEX STUDIED BY MOLECULAR DYNAMICS

Hiroaki Gouda [1], Shuichi Hirono [1]
(School of Pharmaceutical Sciences, Kitasato University[1])

202 Development of conformational search algorithm for proteins

Toshiyuki Kamakura, Hitoshi Gotoh
(Toyohashi University of Technology)

203 Conformational Analyses of a β-Turn Peptide by Brownian Dynamics Simulation

Noriyuki Yamaotsu, Shuichi Hirono
(School of Pharmaceutical Sciences, Kitasato University)

204 Generation of a novel equation for logP estimation using a neural network

Sumie Tajima[1], Kenji Yamagishi[2], Makoto Haraguchi[1], Umpei Nagashima[3]
(Bestsystems Inc.[1], Rikkyo University[2], Grid Technology Research Center[3])

205 Integrated In Silico Screening (III) : Human P450 Prediction Model Construction and Investigation

Masato Kitajima[1] Jose Martin Ciloy[1] Kohtaro Yuta[2]
(Fujitsu kyushu system engineering limited [1] Fujitsu limited[2])

206 Prediction of Protein-Ligand Interactions from molecular, sequence and structure descriptors

Shandar Ahmad and Akinori Sarai

(Kyushu Institute of Technology)

207 Development of a Protein-Ligand Interaction Database, ProLINT, and Its Application to QSAR Analysis

Kouji Kitajima[1] , Shandar Ahmad[1], Hideo Kubodera[2], Shinji Sunada[3], Akinori Sarai[1]

(Kyushu Institute of Technology[1], ZeoGene[2], Mitsubishi Pharma[3])

208 The structure –activity relationship of P-glycoprotein using Chemical Fragment codes

Hiroyuki Hirano[1], Yuko Onishi[1,2], Toshihisa Ishikawa[2]

(GS platZ Co., Ltd. [1], Tokyo Institute of Technology[2])

209 A Functional Study on Genetic Polymorphisms of P-Glycoprotein (ABCB1)

Toshihisa Ishikawa, Aki Sakurai, and Yuko Onishi

(Graduate School of Bioscience and Biotechnology, Tokyo Institute of Technology)

210 A Functional Study on Genetic Polymorphisms of ABCG2

Toshihisa Ishikawa[1], Hideyuki Mitomo[1], Yuko Hagiwara[1], Shiho Kasamatsu[1], Yuko Onishi[1], Akiko Ito[2], Megumi Yoshikawa[2], and Yoji Ikegami[2]

([1]Graduate School of Bioscience and Biotechnology, Tokyo Institute of Technology, [2]Department of Drug Metabolism and Disposition, Meiji Pharmaceutical University)

211 Development of a high-throughput screening system for the substrate specificity of human P-glycoprotein (ABCB1)

Yuko Onishi[1,3], Keisuke Oosumi[2], Hiroyuki Hirano[3], Makoto Nagakura[2], Shigeki Tarui[3], Toshihisa Ishikawa[1]

(Tokyo Institute of Technology[1],Biotec Co.,Ltd.[2],GS PlatZ Co.,Ltd.[3])

212 Homology modeling of human acetylcholine receptor using FAMS Ligand&Complex

Mayuko Takeda-Shitaka, Daisuke Takaya, Hirokazu Tanaka, Mitsuo Iwadate and Hideaki Umeyama

(School of Pharmaceutical Sciences, Kitasato University)

213 Prediction of Inhibition Mechanism of Thymidine Phosphorylase with Water Molecules in Active Site

Yukio Tada [1], Shingo Yano [1], Hideki Kazuno[1], Tsutomu Sato [1], Masakazu Fukushima [1], Tetsuji Asao [1]

(Hanno Research Center, Taiho Pharmaceutical Co., Ltd.[1])

3. 分子生物学における情報計算技法

301 Analysis of Cation-π Interactions in Membrane Protein Structures

M. Michael Gromiha and Makiko Suwa

(Computational Biology Research Center (CBRC),National Institute of Advanced Industrial Science and Technology (AIST))

302 Development of HocDB (Homology-based clustering DataBase), a sequence classification system for database searching

Motokazu Ishikawa[1], Yoshinori Sato[1], Hiroyuki Toh[2]

(Mitsubishi Space Software Co. Ltd[1], Bioinformatics Center, Institute for Chemical Research, Kyoto University[2])

303 Development of Lossless Compression Techniques for Biology Information and its Application for Bioinformatics Database Retrieval

Toshio Modegi

(Research & Development Center, Dai Nippon Printing Co., Ltd.)

304 Bioinformatic Analyses of Transcription Factors

Akinori Sarai[1], Samuel Selvaraj[2], Michael M. Gromiha[3] and Hidetoshi Kono[4]

([1]Kyushu Institute of Technology, [2]Bharathidasan University, India, [3]Computational Biology Research Center, [4]Japan Atomic Energy Research Institute.)

305 Thermodynamic Database for Protein-Nucleic Acid Interactions (ProNIT): Developments in 2003.

M. D. Shaji Kumar[1], Ponraj Prabakaran[2], Hatsuho Uedaira[1], M. Michael Gromiha[3], Kouji Kitajima[1] and Akinori Sarai[1]

(Kyushu Institute of Technology [1], NIH, USA[2], CBRC, AIST[3])

306 Protherm: Thermodynamic Database for Proteins and Mutants

K. Abdulla Bava[1], M. Michael Gromiha[2], Hatsuho Uedaira[1], Koji Kitajima[1],and Akinori Sarai[1]

([1]Kyushu Institute of Technology, [2]Computational Biology Research Center)

308 Identification of Target Genes of the Orphan Nuclear Receptor PPAR

Hiroki Momose [1], Tuguchika Kaminuma[2], Yoshitomo Tanaka[1], 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])

309 Monte Carlo simulation studies on biochemical systems

Ryuzo Azuma[1], Tomoyuki Yamamoto[2], Yoshiki Yamaguchi[1], Akihiko Konagaya[1]

(Genomic Sciences Center, RIKEN[1], School of Knowledge Sci. JAIST[2])

310 A high-speed search method for distributed and federated XML databases

Shin'ichi Tsuji [1,2], Yasuhiko Nakashima[1,2], Kenji Satou[1], Fumikazu Konishi[3], Akihiko Konagaya[3]

(JAIST School of Knowledge Science[1], NEC Software Hokuriku, Ltd.[2], RIKEN Genomic Sciences Center[3])

311 Analysis of Similar Structural Protein with Low Sequence Identity by Coarse-Grained Charge Distribution in Sequence

Kenichiro Imai, Shigeki Mitaku

(Division of Applied Physics Graduate School of Engineering Nagoya University)

312 Development of a structure based protein function prediction

Takeo Asaoka[1], Tadashi Ando[2], Toshiyuki Meguro[3], Ichiro Yamato[4]

(Department of Biological Science and Technology, Tokyo University of Science)

313 A distributed and autonomous job dispatcher for OBIEnv

Yasuhiko Nakashima [1,2], Kenji Satou [1], Shin'ichi Tsuji [1,2], Xavier Defago [3], Akihiko Konagaya [4]

(JAIST School of Knowledge Science [1], NEC Software Hokuriku, Ltd [2],JAIST School of Information Science [3],RIKEN Genomic Sciences Center [4])

314 Identification of Nuclear Receptor Target Genes Related to Drug-Drug Interaction

Yoshitomo Tanaka[1], Tuguchika Kaminuma[2], Hiroki Momose[1], 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])

315 PROMISS: Protein identification support tool for MS analysis data

Aki Hasegawa, Kazumi K. Matsumura, Akihiko Konagaya

(Bioinformatics Group, GSC, RIKEN)

316 Structural Analysis of Metabolic Networks: Format Describing Intermetabolite Atom-Level Connectivity

Jun Ohta

(Okayama University Graduate School of Medicine and Dentistry)

318 Classification of Protein Structures Using PDB-REPRDB system

Noguchi Tamotsu

(Computational Biology Research Center (CBRC), AIST)

320 Feature Representation and Kernel Selection in Prediction of Protein-Protein Interaction Sites Using Support Vector Machine

Gaku Keyakidani[1], Kiyonobu Yokota[1], Yuichiro Nishida[1], Kenji Satou[1,2]

(Japan Advanced Institute of Science and Technology[1],Institute for Bioinformatics Research and Development (BIRD), JST[2])

322 Methods of kinetic parameter estimation from time-courses in E-Cell parameter estimation tools

Shinichi Kikuchi[1], Masahiro Sugimoto[1, 2], Yoshiya Matsubara[1], Mariko Ando[1], and Masaru Tomita[1]

(Laboratory for Bioinformatics, Institute for Advanced Biosciences, Keio University[1], MITSUBISHI SPACE SOFTWARE CO., LTD.[2])

323 Prediction of Biochemical Reactions using Genetic Programming

Masahiro Sugimoto[12], Kikuchi Shinichi[1], Masaru Tomita[1]

(Institute for Advanced Biosciences of Keio University[1],MITSUBISHI SPACE SOFTWARE CO., LTD.[2])

324 Analysis of transmembrane segment for membrane protein discrimination

Toshiyuki Tsuji [1], Shigeki Mitaku[1]

(Division of Applied Physics Graduate School of Engineering Nagoya University [1])

4. ゲノムワイドな解析

401 Development of Method to Predict Protein Function of *Escherichia coli* Using Protein Complex Data

Seira Nakamura [1,6], Rintaro Saito [1], Takeshi Ara [1,2], Aya Itoh [1,2], Md. Arifuzzaman [3,4], Maki Maeda [2], Taku Oshima [2,4], Chieko Wada [2,5], Hirotada Mori [1,2,4], Masaru Tomita [1,7]

(Institute for Advanced Biosciences, Keio University [1], CREST JST [2], NEDO [3],Research and Education Center for Genetic Information, Nara Institute of Science and Technology [4], Institute for Virus Research, Kyoto University [5], Bioinformatics Program, Graduate School of Media and Governance, Keio University [6], Faculty of Environmental Information, Keio University [7])

402 Gene expression analysis using Akaike's Information Criterion

Koji Kadota and Katsutoshi Takahashi

(Computational Biology Research Center (CBRC), AIST)

403 KAREIDMAP: Gene Regulatory Network Analysis Support System

Hironori Mizuguchi[1], Dai Kusui[1], Taku Oshima[2], Shigehiko Kanaya[3] and Hirotada Mori[2,4]

(Internet Systems Research Laboratories, NEC Corporation[1],Research and Education Center for Genetic Information, Nara Institute of Science and Technology[2],Graduate School of Information Science, Nara Institute of Science and Technology[3],Institute for Advanced Biosciences, Keio University[4])

404 Prediction of Motif-Motif Interaction and Protein-Protein Interaction in *Escherichia coli*

Hikaru Kimura[1,3], Seira Nakamura[1,2], Rintato Saito[1], Takeshi Ara[1,4], Aya Itoh[1,4], Md Arifuzzaman[5,6], Maki Maeda[4], Taku Oshima[4,6], Chieko Wada[4,7], Hirotada Mori[1,4,6], Masaru Tomita[1,3]

(Institute for Advanced Biosciences, Keio University[1], Bioinformatics Program, Graduate School of Media and Governance, Keio University[2], Faculty of Environmental Information, Keio University[3], CREST, JST[4], NEDO[5], Research and Education Center for Genetic Information, Nara Institute of Science and Technology[6], Institute for Virus Research, Kyoto University[7])

405 Fundamental examination of data evaluation for Yeast cDNA microarray

Satomi MIZUKAMI[1], Yoshiteru SUZUKI[2], Hitoshi IWAHASHI[3]

(Advanced Industrial Science and Technology (NEDO) [1],Advanced Industrial Science and Technology[2],Human Stress Signal Research Center[3])

406 Transcriptome profiling and cluster analysis of *Saccharomyces cerevisiae* under environmental stress conditions.

Yoshiteru Suzuki , Kim Hyun-Ju , Yuko Momose , Emiko Kitagawa , Takayuki Honma , Sophon Shirisatta , Sakiko Kurita , Megumi Kojima , Parveen Meher , Shinzou Kimura , Junko Takahasi , Hitoshi Iwahashi

(National Institute of Advanced Industrial Science and Technology (AIST))

407 The acquisition of freezing/thawing tolerance was caused by respiration activity in mitochondria

Yoshinori Murata, Hitoshi Iwahashi, and Syuu-ichi Oka

(International Patent Organism Depositary AIST)

408 Constructing Reliable Protein Complex Data of *Saccharomyces cerevisiae*

Rintaro Saito, Masaru Tomita

(Institute for Advanced Biosciences, Keio University)

409 Assistance tool for MS/MS shotgun analysis

Chihiro Higuchi , Toshiyuki Mikami , Kazunori Yanagi , Jun Sakai , Shinichi Kojima , Masaharu Kanaoka

(Genomic Science Laboratories, Sumitomo Phamaceuticals Co., Ltd.)

410 cDNA microarray for human skeletal muscles to understand the molecular mechanism of myogenesis and myostatin effect

Satoru Noguchi[1, 2], Rumi Kurokawa[1, 2], Masako Fujita[1, 2], Toshifumi Tsukahara[2, 3], Atsumi Tsujimoto[2, 4], Ichizo Nishino[1, 2]

(National Institute of Neuroscience, National Center of Neurology and Psychiatry[1], CREST JST[2], Japan Advanced Institute of Science and Technology[3], DNA Chip Research Inc[4].)

411 Profiling of genome-wide expression of protein translocation defect of *Escherichia coli*

Hisayo Shimizu[1], Hajime Tokuda[2], Hitoshi Iwahashi[1], Syuichi Oka[1]

(AIST International Patent Organism Depositary [1], Institute of Molecular and Cellular Biosciences [2])

412 Development of expression profile analysis tool SOSUIarray which is focused on transmembrane proteins

Naoyuki Asakawa[1], Shigeki Mitaku[2]

(Tokyo University of Agriculture and Technology[1], Nagoya University[2])

413 Ranking of Biological Pathway Using GSCope and Microarray Data

Yoshikazu Hasegawa[1], Katsura Hirosawa[1], Naoki Okamoto[2],Tetsuro Toyoda[1] and Akihiko Konagaya[1]

(Bioinformatics Group, GSC, RIKEN[1], NEC Infomatec Systems Ltd[2])

414 Classification of stress-induced genomic expression profiles

Yuko Momose[1], Hitoshi Iwahashi[1], Shu-ichi Oka[1]

(The National Institute of Advanced Industrial Science and Technology (AIST) [1])

416 How to choose best probe set for oligo DNA microarrays?

Mikihiko Nimura [1], Masato Inoue[1], Yasuyuki Hayashi[1], Todd Richmond[2], Michael Hogan[2], Steve Smith[2], Roland Green[2]

(GeneFrontier Corporation [1], NimbleGen Systems, Inc.[2])

417 Development of Magtration® System 8Lx

Tomoyuki Hatano, Yuriko Tojo, Hironobu Satoh, Yoshinao Hirahara, Masaaki Takahashi, Kimimichi Obata, Hideji Tajima

(Precision System Science Co., Ltd., Matsudo, Japan)

418 Method for identification of transcription regulatory regions by comparative genomics

Jiro Araki, Takeaki Taniguchi, Takehiko Ito

(Mitsubishi Research Institute Inc.)

419 Automatic generation of cell-wide pathway model from complete genome

Kazuharu Arakawa[1,2], Yohei Yamada[1,3], Hiromi Komai[1,3], Kosaku Shinoda[1,4], Yoichi Nakayama[1,3], Masaru Tomita[1,3]

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420 G-language Genome Analysis Environment Version 2

Kazuharu Arakawa[1,2], Ryo Hattori[1,3], Yohei Yamada[1,3], Yusuke Kobayashi[1,3], Hayataro Kouchi[1,3], Atsuko Kishi[1,3], Masaru Tomita[1,3],

(Institute for Advanced Biosciences, Keio University[1], Bioinformatics Program, Graduate School of Media and Governance[2], Department of Environmental Information[3])

421 Homology search of proteins using non-additive entropy

Takahashi Koichi, Nakamura Naoki

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422 More Conserved Upstream Sequences for Transcription Factor Genes and its Evolutionary Implication

Hisakazu Iwama[1,2] and Takashi Gojobori[1,2]

([1]National Institute of Genetics, [2]National Institute of Advanced Industrial Science and Technology)

5. 医薬品開発と有害事象研究基盤

501 *Ki* Bank: A Database for Molecular Interaction Analysis between Proteins and Chemicals

Junwei Zhang[1], Masahiro Aizawa[1], Kenji Onodera[1], Shinji Amari[1], Yoshio Iwasawa[2] and Kotoko Nakata[3]

([1]Collaborative Research Center of Frontier Simulation Software for Industrial Science, Institute of Industrial Science, University of Tokyo; [2]AdvanceSoft Corporation; [3]Division of Safety Information on Drug, Food and Chemicals, National Institute of Health Sciences)

502 Analysis and Prediction of Drug Excretion into Human Breast Milk (2nd) - Additional Analysis Including Hydrophilic Compounds -

Takashi Fujiwara, Yuki Hibino, Masaru Kihara, Aiko Yamauchi, Hiroshi Chuman

(Graduate School of Pharmaceutical Sciences, The University of Tokushima)

503 *In situ* Measurement for Apoptotic Carcinoma Cells Using by a Photon Correlation Spectroscopy

Mayu Nakamura, Takahito Kawamura, Shintaro Obara, Hiroshi Takano and Masayuki Itoh

(Department of Chemical Engineering and Materials Science, Doshisha University)

504 Kinetic simulation of signal transduction system in hippocampal long-term potentiation with dynamic modeling of protein phosphatase 2A

Shinichi Kikuchi[1], Kenji Fujimoto[1], Noriyuki Kitagawa[1], Taro Fuchikawa[1], Michiko Abe[1], Kotaro Oka[1, 2], Kohtaro Takei[1, 3], Masaru Tomita[1]

(Laboratory for Bioinformatics, Institute for Advanced Biosciences, Keio University[1], Dept. of Biosciences and Informatics, Faculty of Science and Technology, Keio University[2], Dept. of Molecular Pharmacology and Neurobiology, Yokohama City University School of Medicine[3])

505 Assessment of Intestinal First Pass Effect by TMF Model: A Study on Metoprolol, CYP2D6 Substrate

Takashi Mizuma[1], Masahiro Hayashi[1]
(Tokyo University of Pharmacy and Life Science [1])

506 Structural Search with Pharmacological Information in 3D Pharmaceutical Structure Database (3DPSD)

Manabu Watanabe[1], Kaori Kurata[1], Masaki Hamada[1], and Akira Dobashi[1]
(Tokyo University of Pharmacy and Life Science, School of Pharmacy[1])

507 Research on Construction and Practical Use of Pediatric Dosage Database System which Assists Prescribing and Inspection

Masaharu Terasawa[1] Mitsuhiro Okazaki[2] Miki Kaneuchi[2] Hiromichi Yukawa[3] Noriaki Tamura[3] Yoshiyuki Kosugi[1] Naonori Kohri[2] Yukitoshi Hayase[2] Tatsuo Nagasaka[1]
(Tokyo University of Pharmacy and Life Science[1] Hokkaido College of Pharmacy[2] JR East Japan Information Systems Company[3])

508 Data Evaluation and Investigation for Ames Mutagenicity Prediction and QSAR Analysis: Trend Analysis by Lipinski Parameters and Chemical Parameters

Katsuhiko Sawatari[1], Yoshifumi Nakanishi[1], Kohtarou Yuta[2], Taijiro Matsushima[3]
(National Institute of Industrial Health[1], Fujitsu Ltd.[2], Japan Bioassay Research Center[3])

6. 疾病モデル

601 DRY WET Hybrid Supporting System for Genomic Translational Research (Hybrid-TRS)

Jun Nakaya[1], Akira Sasaki[1], Hideji Ohtani[2], Reiko Tachino[3], Takako Sakamoto[1], Tetsuo
(Institute of Medical Science of the Tokyo University [1], Fujitsu[2], Tokyo Clinical Research Center [3])

602 Knowledge Architecture for Bridging Genomic Science and Clinical Medicine (KAB)

Jun Nakaya[1], Koji Sasaki[2], Akira Sasaki[1], Takako Sakamoto[1], Tsuguchika Kaminuma[3], Tetsuo Shimizu[1]
(Institute of Medical Science of the University of Tokyo [1], AdIn Research Inc.[2], Biodynamics Inc. [3])

603 Evidence Based Knowledge Structure for Complimentary and Alternative Medicine (EBKS-CAM)

Jun Nakaya[1], Yoshinori Ohtsuka[2], Yuko Agishi[3], Koji Sasaki[4], Tsuguchika Kaminuma[5], Tetsuo Shimizu[1]
(Institute of Medical Science of the University of Tokyo [1], Hokkaido University[2], Health and Resort Research Institute [3], AdIn Research Inc.[4], Biodynamics Inc.[5])

604 Functional Analysis of Mammalian Cell Cycle Using a Computational Model of Hybrid Petri Net

Shuji Kotani [1] , Takashi Yoshioka [2] , Kaoru Takahashi [1] , Akihiko Konagaya [1]
(RIKEN Genomic Sciences Center (GSC) [1], NTT DATA Corporation [2])

605 Molecular Knowledge Base for Syndrome X

Tsuguchika Kaminuma[1], Masumi Yukawa[2], Naomi Komiyama[2], Hiroki Momose[3], Yoshitomo Tanaka[3], Hiroshi Tanaka[3]
(Biodynamics Inc.[1], Chem-Bio Informatics Society[2], Medical Research Institute, Tokyo Medical and Dental University[3])

606 An Electrophysiological Simulation Model of the Myocardial Cell Using E-CELL System

Sayaka Ishinabe [1,2], Yasuhiro Naito [1,3], Motohiro Yoneda [1,2], Katsuya Kawai [1,2], Shoko Miyamoto [1,2], Shinobu Kuratomi [4], Nobuaki Sarai [4], Satoru Matsuoka [4], Akinori Noma [4], Masaru Tomita [1,3]
(Institute for Advanced Biosciences, Keio University [1], Graduate School of Media and Governance, Keio University[2], Department of Environmental Information, Keio University [3], Department of Physiology and Biophysics, Graduate School of Medicine, Kyoto University [4])

7. その他—新規技術

701 Methylation profile of CpG islands in promoter region for the genes related pancreatic carcinogenesis

Takazumi Kozaki[1, 4], Johji Imura[2], Haruo Iguchi[3], Aki Hasegawa[1], Masafumi Yohda[4] and Ryuji Kawaguchi[1]
(Genomics Research Institute, SRL, Inc[1], Department of Surgical and Molecular Pathology, Dokkyo University of School of Medicine[2], Department of Clinical Research, National Kyusyu Cancer Center[3], Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology[4])

702 Development of a new detection device for micro-beads using optical fibers

Kazumi Sawakami[1], Hatsumi Abe[1], Osamu Segawa[1], Masaaki Takahashi[1], Hideji Tajima[1], Ken Tsukii[2], Toru Takahashi[2], Xu Jie[2], Sadayuki Toda[3], Masayuki Machida[4]
(Precision System Science Co., Ltd.[1], The Furukawa Electric Co., LTD.[2], FI-Techno Co., Ltd.[3], AIST RCG[4])

703 Hierarchical Stratification of Protein Protein Interaction Network

Takeshi Hase, Yasuhiro Suzuki, Souichi Ogishima, Sou Nakagawa, Hiroshi Tanaka
(Dept. of Bioinformatics, Graduate School of Tokyo Medical and Dental University)

704 An efficient way to perform DDBJ homology search

Takashi Miyajima[1], Yutaka Kawarabayasi[2]
(TM Software, Inc.[1], AIST[2])

705 Expression and characterization of an extracellular molecular chaperone, Clusterin

Yuko Arie, Nobuo Misawa, Ryo Iizuka, and Masafumi Yohda
(Dept. of Biotechnol., Tokyo Univ. of Agric. & Technol.)

706 Structure and function of Hsp42 from Saccharomyces cerevisiae

Maya Hirose[1], Keisuke Usui[1], Nriyuki Ishii[2], Masafumi Yohda[1]
(Tokyo University of Agriculture and Technology [1], Nat. Inst. of Adv. Ind. Sci. and Tech[2])

707 Effect of ATP binding on the conformation of archaeal group II chaperonin

Ryo IIZUKA[1], Takao YOSHIDA[2], Yasuhito SHOMURA[3], Kunio MIKI[3], Tadashi MARUYAMA[4], Tomonao INOBE[5], Kunihiro KUWAJIMA[5], Masafumi YOHDA[1]
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708 Structural & functional characterization of ClpC from *Bacillus subtilis*

Keisuke UCHIDA[1], Ryo IIZUKA[1], Noriyuki ISHII[2], Masafumi YOHDA[1]
([1]Dept. of Biotechnol., Tokyo Univ. of Agric. & Technol., [2]JBIRC, AIST)

709 Development of the Total System for Molecular Design

Tetsuhiro Suzukawa, Soichiro Mizobuchi, Masamoto Arakawa, Kimito Funatsu
(Toyohashi University of Technology)

710 Development of a molecular memory system based on hairpin DNA

Masahiro Takinoue[1], Akira Suyama[1, 2]
(Institute of Physics University of Tokyo[1], JST CREST[2])

711 SYCRP1-DNA binding mechanism studied through thermodynamic and structural data.

Katsumi Omagari[1] , Hidehisa Yoshimura[1], Mitsunori Takano[1] , Masayuki Ohmori[1], Akinori Sarai[2], Akira Suyama[1]
(Univ. of Tokyo[1], Kyushu Inst. of Tech.[2])

712 Roles of the helical protrusion of the group II chaperonin

So Sena[1], Ryo Iizuka[1], Tomonao Inobe[2], Kunihiro Kuwajima[2], Masafumi Yohda[1]
(Tokyo University of Agriculture and Technology [1], Tokyo University[2])

713 Development of Bio-Strand System for multiple samples/items analysis

Yukiko Miyashita[1], Junko Asahina[1], Osamu Segawa[1], Yuriko Tojo[1], Masaaki Takahashi[1], Hideji Tajima[1], Masafumi Yohda[2]
(Precision System Science Co., Ltd.[1], Tokyo University of Agriculture and Technology[2])

714 Development of SNPs detection method using MagSNiPer

Fumiko Kakihara[1, 2], Akiko Katsura[1], Junichi Akutsu[1], Mina Okochi[1], Yuriko Tojo[3], Hideji Tajima[3], Masafumi Yohda[1], Setsuo Hasegawa[2]

(Tokyo University of Agriculture and Technology [1], Sekino Clinical Pharmacology Clinic[2], Precision System Science[3])

715 Fluorescence detection and kinetic analysis of interaction between *Pyrococcus* prefoldin and substrate

Tamotsu Zako[1], Ryo Iizuka[2], Mina Okochi[2], Taro Ueno[1], Masafumi Yohda[2], Takashi Funatsu[1]

(Waseda University[1], Tokyo University of Agriculture and Technology [2])

716 OBIGrid application of Blast service in the hetero cluster of parallel

Fumikazu KONISHI[1], Ryo UMETSU[1], Akihiko KONAGAYA[1]

(RIKEN Genomic Sciences Center[1])

717 Complex dissociation and the role of N-terminal region of sHsp from *Sulfolobus tokodaii* strain 7

Keisuke Usui[1], Omer Faruk Hatipoglu[1], Noriyuki Ishii[2], Masafumi Yohda[1]

(Tokyo University of Agriculture and Technology [1], National Institute of Advanced Industrial Science and Technology [2])

718 Simulation of apoptosis based on the labeling problem

Akira Tachikawa

(Department of Biomedical Engineering, Graduate School of Medicine, University of Tokyo)

719 Application of Drug Interaction Ontology (DIO) for Possible Drug-drug Interactions

Sumi Yoshikawa[1, 2], Kenji Satou [1], Akihiko Konagaya[2]

(School of Knowledge Science, Japan Advanced Institute of Science and Technology (JAIST)[1], Genomics Science Center (GSC), RIKEN (The Institute of Physical and Chemical Research) [2])

720 Comprehensive analysis of yeast DNA-binding proteins by phage display and DNA microarray

Hiroko Hagiwara[1], Sumiko Kunihiro[1], Midori Yamamoto[1], Keiichi Nakajima[1], Motoaki Sano[1], Kumiko Takase[1], Haruhiko Masaki[2], Ichiro Kuwabara[3], Ichiro Maruyama[3], Masayuki Machida[1]

([1]AIST, [2]Univ. of the Tokyo, [3]The Scripps Res. Inst.)

721 A Discrete Mathematical Model of Inflammatory Response

Yasuhiro Suzuki[1,2], Michihiko Koeda[1], Hiroshi Tanaka[1]

(Tokyo Medical and Dental University[1], Advanced Telecommunications Research inst.[2])