LIST OF POSTERS

Poster Session I

November 30, 2010 13:40-15:50

Odd Poster Numbers Room 305 P001~P045 Room 207 P047~P091

Poster Session II

December 1, 2010 13:40-15:50

Even Poster Numbers Room 305 P002~P046 Room 207 P048~P090

Folding study of outer surface protein A

Koki Makabe, Takashi Nakamura and Kunihiro Kuwajima Okazaki Institute for Integrative Bioscience

P002

Solvent effect on structural stability of human telomere

*Yutaka Maruyama¹;Taku Matsushita2;Masahiro Ohgidani²;Masayuki Takeda²;Osamu Tanoue²;Ryuichi Ueoka²;Fumio Hirata¹

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P003

Database analysis of protein structural changes upon ligand binding

Takayuki Amemiya^{1,2}; *Akinori Kidera^{1,3} 1Yokohama City University; 2School of Informatics, Nagoya University; 3Riken Institute

P004

Leu628 of the KIX Domain of CBP is a Key Residue for the Interaction with the MLL Transactivation Domain

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P005

Graded enhancement of p53 binding to CREB-binding protein (CBP) by multisite phosphorylation

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Protein Interactions Monitored by NMR: Intrinsically Disordered p53 Transactivation Subdomains Interact with the TAZ2 Domain of CBP at Two Sites

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P007

Modulation of the Altered Functional Characteristics of Circularly Permuted GroEL through the Introduction of Disulfide Bonds

*Tomohiro Mizobata^{1,2}; Tatsuya Uemura²; Toshifumi Mizuta²; Yusuke Yakushiji¹; Kazuhiro Isaji¹; Takuya Okada¹; Kunihiro Hongo^{1,2}; and Yasushi Kawata^{1,2}

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P008

Probing the roles of conserved arginine-44 of Escherichia coli dihydrofolate reductase in its function and stability by systematic sequence perturbation analysis

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P009

Specificity and nonlinearity in large-amplitude motion of allosteric proteins

Wenfei Li; *Shoji Takada Graduate School of Science, Kyoto University

P010

Free energy landscape analysis of biomolecules by massive parallel multi-scale simulation

*Ryuhei Harada^{1,2}; Akio Kitao^{1,2}
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Challenge to reproduction of hyper-mobile water around monovalent ions: Classical molecular dynamics study

Ikuo Kurisaki¹; Takuya Takahashi^{1,2}

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P012

Alteration of lipid constituent in cancer cell membrane induced by hybrid liposome

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P013

Protein salting-out observed at an air-water interface

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P014

Ensemble modeling of p53 intrinsically disordered N-terminal domain by combining multi-scale simulations with NMR experiments

*Tsuyoshi Terakawa¹; Shoji Takada¹ 1Department of Biophysics, Kyoto University

P015

Elucidation of protein fluctuation by relaxation dispersion NMR spectroscopy and water-amide proton exchange

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Fluctuation Controls Enzymatic Activity of Staphylococcal Nuclease

Hironari Kamikubo; Shigefumi Tadokoro; *Mikio Kataoka Graduate School of Materials Science, Nara Institute of Science and Technology

P017

Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation

*Xin-Qiu Yao¹; Hiroo Kenzaki¹; Shoji Takada^{1,2} 1Department of Biophysics, Kyoto University; 2CREST, Japan Science and Technology Agency

P018

Emission Spectral Analysis of Europium(III) Probes Attached to Proteins

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P019

Large fluctuations of DNA bases induced by binding to homologous pairing proteins

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P020

Lateral Diffusion of Phospholipid Molecules Separated from the Rotational and the Translational Diffusion of a Fluid Bilayer Vesicle

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Temperature effect on the fluctuation of titin I27 domain: the DHS analysis of the mechanical unfolding free energy landscape

*Yukinori Taniguchi¹;Zu Thur Yew²;Emanuele Paci²;Masaru Kawakami¹

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P022

Monomer-dimer fluctuation of transmembrane helices as detected by single-molecule fluorescence microscopy

*Yoshiaki Yano; Ryota Kitani; Katsumi Matsuzaki Graduate School of Pharmaceutical Sciences, Kyoto University

P023

Design of novel metal-binding proteins based on influenza M2 protein

*Yoshihiro Iida¹; Atsuo tamura¹ 1Department of Chemistry, Graduate School of Science, Kobe University

P024

Localization of amyloid-destabilizing mutations in the N-terminal domain of Rnq1 in Saccharomyces cerevisiae

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P025

Application of fluorescence lifetime correlation measurements to biological molecules

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Stabilization of BPTI-[5,55] through decrease of local backbone fluctuations and development of hetero-microseeding for crystallizing low-stability proteins

Yutaka Kuroda, Mohamed M Islam, Kei Kobayashi Dept of Biotech and life Science, TUAT

P027

Clustering of Lipid Rafts in Plasma Membranes by Hybrid Liposomes for Leukemia Cells Leading to Apoptosis

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P028

Detecting coupled motions in protein with Molecular Dynamics simulation

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P029

Anomalous Diffusion in Supported Planar Lipid Bilayers on Nano-Structured Oxide Substrates

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P030

Fluctuation and function of polyglutamine tract binding protein-1

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MD simulations and QM calculations of water around small solute

Takuya Takahashi^{1,2}; Ikuo Kurisaki¹

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P032

Calorimetric Study of Conformational Fluctuation of Alkyl Chain in Lamellar Phase of Monoacylglycerol/water systems

Yasuhisa Yamamura, Shin Nakada, Maika Iwami, Airi Katagiri, Syuma Yasuzuka, Kazuya Saito

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P033

Contribution of an arginine residue of Zif268 zinc finger on the structure and DNA binding

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P034

The role of the cytoplasimic domain in pH-dependent gating by the KcsA channel

*Minako Hirano^{1,2}; Toru Ide^{1,2} 1RIKEN; 2Graduate School of Frontier Biosciences, Osaka University

P035

Novel method for saturation mutagenesis of proteins using cell-free translation system

*Takayoshi Watanabe; Toshiya Mineura; Takahiro Hohsaka School of Materials Science, Japan Advanced Institute of Science and Technology

Effect of cations on G-quadruplex structure and fluctuation of telomeric DNA

Taku Matsushita¹; Masahiro Ohgidani¹; Masayuki Takeda¹; Osamu Tanoue¹; Yutaka Maruyama²; Fumio Hirata²; Ryuichi Ueoka¹

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P037

Structural analysis on folding intermediate of srcSH3

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P038

DYNAMIC EQUILIBRIUM OF LYS48-LINKED DI-UBIQUITIN IN SOLUTION ASSESSED BY NMR

*Takashi Hirano¹; Olivier Serve²; Maho Yagi^{1,2}; Tsunehiro Mizushima¹; Koichi Kato^{1,2}
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P039

Conformational Fructuations Associated with Variable Domains of Pathogenic and Nonpathogenic Immunogloblin Light Chains

*Daizo Hamada; Tetsuyuki Abe; Kyohei Ikeda Division of Structural Biology (GCOE), Department of Biochemistry & Molecular Biology, Graduate School of Medicine, Kobe University

P040

Fluctuation of Ion and Water Flux through the KcsA Potassium Channel

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Effect of pressure on beta-hairpin peptides

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P042

Property of Glycan-processing Enzyme under Extracellular Matrix Conditions

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P043

EVALUATION OF AGING-RELATED DISEASES BY N-LINKED GLYCANS UNDER MOLECULAR CROWDING CONDITIONS

*Miho Tada¹; Hikaru Matsushima¹; Yukishige Ito^{2,3}; Kiichiro Totani¹

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P044

Direct manipulation of a single potassium channel gate with an atomic force microscope probe

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and Industrial Research

P045

Remarkable Therapeutic Effects of Hybrid Liposomes on the Growth of Gastric Carcinoma along with Apoptosis

*Hideaki Ichihara, Yusuke Matsuoka, Yuji Komizu, Yoko Matsumoto, Ryuichi Ueoka Division of Applied Life Science, Graduate School of Engineering, Sojo University

Time-resolved observation of protein-protein interaction between blue-light receptor PixD and response regulator PixE

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P047

Fluctuation in the mechanism of HIV protease inhibitors between HIV protease and proteasome

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P048

Folding of a helical miniprotein studied by multicanonical replica-exchange molecular dynamics simulations

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P049

Kinetic intermediates of beta2-microglobulin fibril elongation probed by pulse-labeling H/D exchange combined with NMR analysis

*Eri Chatani^{1,2}; Tsuyoshi Konuma¹; Reina Ohnishi¹; Masanori Yagi¹; Kazumasa Sakurai¹; Takahisa Ikegami¹; Hironobu Naiki³; Yuji Goto¹

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P050

Laser-induced Propagation and Destruction of Amyloid beta Fibrils

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THE MOLTEN GLOBULE STATE AND ITS BIOLOGICAL FUNCTION IN $\,\,\alpha$ -LACTALBUMIN

*Takashi Nakamura^{1,2}; Koki Makabe^{1,2,3}; Tomoyasu Aizawa⁴; Keiichi Kawano⁴; Makoto Demura⁴; Kunihiro Kuwajima^{1,2,3} 10kazaki Institute for Integrative Bioscience; 2Institute for Molecular Science; 3Department of Functional Molecular Science, The Graduate University for Advanced Studies; 4Division of Life Science, Graduate School of Life Science, Hokkaido University

P052

Microsecond-resolved time traces of protein folding by single-molecule fluorescence detection

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P053

Time-resolved study on the protein-protein interaction of Anabaena sensory rhodopsin

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P054

An application of RISM method incorporating intramolecular fluctuation

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P055

Comparison of DNA hydration patterns obtained using two distinct computational methods, MD simulation and 3D-RISM theory

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Sequence dependent kinetics of hydration water molecules in the minor groove of DNA

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P057

Conversion from BLUF Protein to LOV Protein?

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P058

Pressure-induced fluctuations of local protein structures: Generalized-ensemble simulation study

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P059

Protein Fluctuation Revealed by Pressure Dependence of Intramolecular FRET

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P060

FRET analysis of protein structures by double-incorporation of nonnatural amino acids

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The investigation of the relationship between non-local interaction and the effect of single alanine insertion in staphylococcal nuclease

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P062

Classification of the functional element of dihydrofolate reductase by the systematic alanine insertion

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P063

Bacterial $\ f$ lagellar filament: A metastable structure in polymorphic transformation

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P064

Effect of partial fluorination of hydrophobic chains in phosphatidylcholine on structure and function of bacteriorhodopsin reconstituted into artificial lipid vesicles

*Masashi Sonoyama¹; Masaru Yoshino¹; Takashi Kikukawa²; Yasunori Yokoyama³; Toshiyuki Takagi⁴; Hiroshi Takahashi¹; Makoto Demura²; Teruhiko Baba⁴; Toshiyuki Kanamori⁴ 1Department of Chemistry and Chemical Biology, Gunma University; 2 Faculty of Advanced Life Science, Hokkaido University; 3Department of Applied Physics, Nagoya University; 4Research Center for Stem Cell Engineering, AIST

P065

Chiroptical studies of amyloid-forming proteins in condensed phase and the interactions with membranes

*Reiko Kuroda; Takunori Harada; Natsuyo Asano; Ishrat Jahan Department of Life Sciences, Graduate School of Arts and Sciences, The University of Tokyo

Probing the collective mode of proteins using low-frequency Raman spectroscopy

*Taku Muneda; Ryuichi Wada; Kato Minoru Department of Science and Engineering, Ritsumeikan University

P067

light induced large structural fluctuation of BLUF protein TePixD revealed by high-pressure TG method

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P068

Paramagnetic NMR approach to the analysis of conformations and dynamics of N-glycans

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Structural Biology, Max Planck Institute for Biophysical Chemistr

P069

Spectroscopic characterization of inter-molecular interaction of amyloid β promoted on GM1 clusters

Maho Yagi^{1,2}; *Koichi Kato^{1,2}
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P070

pH-INDUCED FOLDING AND UNFOLDING OF HORSE APOMYOGLOBIN IN THE SUBMILLISECOND TIME RANGE

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HIGH-ENERGY STATE MUTANT OF UBIQUITIN

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P072

FRET analysis of structural changes in Staphylococcal nuclease

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P073

Measurements of Loop Formation in the Denatured State of Staphylococcal Nuclease

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P074

Photoreaction dynamics of photosensor protein: Phototropin2 LOV1 domain

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P075

Multi-scale simulation of a molecular motor actomyosin: toward understanding the weak-to-strong binding transition

*Kei-ichi Okazaki; Jun Ohnuki; Takato Sato; Mitsunori Takano Graduate School of Advanced Science and Engineering, Waseda University

Volume fluctuation of proteins as revealed by isothermal compressibility

*Tadashi Kamiyama Department of Chemistry, Kinki University

P077

FUNCTIONAL ANALYSIS OF POLYAMINE-LIPID/DNA COMPLEX (LIPOPLEX) AS GENE CARRIER: RELATIONSHIP BETWEEN METAMORPHOSIS OF LIPOPLEX AND ITS FUNCTION

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P078

Molecular Recognition Controlled by a Detailed Balance: A Host-Guest Mechanism for 25,26,27,28-Tetramethoxycalix[4]arene in Sodium and Potassium Perchlorate Salt Solutions

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P079

Solvent penetration in the photoactive yellow protein studied by 3D-RISM theory

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P080

Dissecting a bimolecular process of ATP binding to the chaperonin GroEL

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Low-frequency dynamic of ATP and its related compounds studied by terahertz time-domain spectroscopy

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P082

New approach to investigate the molecular recognition of protein toward structure-based drug design based on 3D-RISM theory

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P083

The statistical mechanics study of potassium channels.

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P084

Cytochrome c polymerization by successive domain swapping at the C-terminal helix

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P085

Local Solvation Thermodynamics Analysis of Amyloid-Beta Protein Misfolding

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Effect of secondary structural formation on low-frequency dynamics of poly-L-glutamic acid studied by terahertz time-domain spectroscopy

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P087

Temperature dependence of vibrational dynamics in aqueous solutions

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P088

Vibrational Dynamics of [RuCl5(NO)]2- in Aqueous Soution Studied by Nonlinear Infrared Spectroscopy

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P089

Low-frequency Dynamics of Myoglobin by Terahertz Time-Domain Spectroscopy

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P090

Solvation dynamics in aqueous solution by fluorescence up-conversion method: deuterium effect, temperature dependence, probe molecule dependence

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Low-frequency dynamics of biological molecules studied by terahertz time-domain spectroscopy

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