

The 62nd Annual Meeting of the Nuclear Magnetic Resonance Society of Japan (2023)

Period: November 7 (Tue) – 9(Thu), 2023

Venue: **Yokosuka Arts Theatre**

Hon-cho 3-27 Yokosuka, Kanagawa 238-0041

Day 1 (Tue. 7th Nov.)

9:45 - 9:55 Opening Remarks by Prof. Toshimichi Fujiwara
(President of the Nuclear Magnetic Resonance Society of Japan)

Presentation I [Large Hall]

10:00 - 11:00 Chairperson: Jun Kikuchi

10:00 - 10:20

1L01 Development of evaluation method for minute NMR spectral changes

○Kyoko Furuita¹, Chojiro Kojima^{1,2}

1 *Institute for Protein Research, Osaka University*

2 *Graduate School of Engineering Science, Yokohama National University*

10:20 - 10:40

1L02 Elucidation of structural dynamics of a cyclic multi-domain protein by an integrated approach of NMR relaxation experiments and coarse-grained MD simulations

○Daichi Morimoto¹, Tomoki Sorada¹, Erik Walinda², Masahiro Shirakawa¹, Kenji Sugase³

1 *Graduate School of Engineering, Kyoto University*

2 *Graduate School of Medicine, Kyoto University*

3 *Graduate School of Agriculture, Kyoto University*

10:40 - 11:00

1L03 ¹H, ¹³C, ¹⁵N NMR and DFT calculation studies on complex formation mechanism of zinc(II) ion with ethylenediamine in ionic liquid [C2mIm][TFSA]

○Mikio Maseda¹, Toshiyuki Takamuku²

1 *Analytical Research Center for Experimental Sciences, Saga University*

2 *Department of Chemistry and Applied Chemistry, Faculty of Science and Engineering, Saga University*

11:00 - 11:10 Break Time

Company Presentation [Large Hall]

11:10 - 11:40 Chairperson: Hikaru Momose

11:10 - 11:25

1L04 Evaluation of the surface (adsorption) structure of pigment dispersion using DIRECTION technique

○Ryu Koike, Mieko Koiso, Mariko Kouyama, Yuji Tamura, Atsushi Miyakawa, Akira Kasai
Advanced Analysis & Research Center, DIC Corporation

11:25 - 11:40

1L05 Development of a 1.01 GHz NMR system and its application to the high-resolution NMR in solution

○Junpei Hamatsu¹, Fumihiro Yamazaki², Kenichi Hachitani¹, Toshio Yamazaki³,
Yoshinori Yanagisawa^{3,4}

1 *Group 1, NM Research and Development Department, NM Business Unit, JEOL Ltd.*

2 *Team 1, Electrical Design Group, NM Design Department, NM Business Unit, JEOL Ltd.*

3 *Next-Generation Magnet Development Collaboration Unit, Center for Biosystems Dynamics Research, RIKEN*

4 *RIKEN-JEOL Collaboration Project, RIKEN Industrial Co-creation Program, RIKEN-JEOL Collaboration Project, Cluster for Science, Technology and Innovation Hub, RIKEN*

11:40 - 11:45 Break Time

11:45 - 12:45 General Meeting of the NMR Society of Japan

12:45 - 13:30 Lunch

13:30 - 15:30 Poster Session I (**even number** -xx, 1P-xx & YP-xx) [Small Hall]

Presentation II [Large Hall]

15:30 - 16:30 Chairperson: Kazuyuki Takeda

15:30 - 15:50

1L06 Real time NMR spectroscopy of inorganic pyrophosphatase catalysis using bullet-DNP

○Jun Fukazawa¹, Yuki Mochizuki^{1,2}, Masahiro Kitagawa^{1,2}, Makoto Negoro¹,
Akinori Kagawa^{1,3}, Natsuko Miura⁴

1 *Center for Quantum Information and Quantum Biology, Osaka University*

2 *Graduate School of Engineering Science, Osaka University*

3 *Premium Research Institute for Human Metaverse Medicine, Osaka University*

4 *Graduate School of Agriculture, Osaka Metropolitan University*

15:50 - 16:10

1L07 Optimal-control-based C β chemical shift encoding for solid proteins

○Hajime Tamkai¹, Yoh Matsuki²

1 *Institute for Protein Research, Osaka University*

2 *Center for Quantum Information and Quantum Biology, Osaka University*

16:10 - 16:30

1L08 Real-time monitoring of the structural transition of Bombyx mori liquid silk under pressure by solid-state NMR

○Yu Suzuki¹, Shota Morie¹, Hideyasu Okamura¹, Tetsuo Asakura², Akira Naito²
1 *Department of Applied Chemistry and Biotechnology, Graduate School of Engineering, University of Fukui*
2 *Department of Biotechnology, Tokyo University of Agriculture and Technology*

16:30 - 16:40 Break Time

Presentation III [Large Hall]

16:40 - 18:00 Chairperson: Chojiro Kojima, Takahisa Ikegami

16:40 - 17:00

1L09 Structural study on a chaperone complex for protein unwinding

Haojie Zhu¹, Soichiro Kawagoe¹, Hiroyuki Kumeta³, Koichiro Ishimori¹, ○Tomohide Saio¹
1 *Institute of Advanced Medical Sciences, Tokushima University*
2 *Faculty of Advanced Life Science, Hokkaido University*
3 *Department of Chemistry, Faculty of Science, Hokkaido University*

17:00 - 17:20

1L10 Non-detergent sulfobetaines enable solution NMR measurements of unstable protein complexes

○Kaori Wakamatsu¹, Rinka Sugawara¹, Ibuki Busujima¹, Mai Morooka¹, Toshiyuki Kohno², Kazuo Hosoda¹, Shin-ichi Terawaki³
1 *Division of Molecular Science, Gunma University*
2 *Kitasato University School of Medicine*
3 *Proteo-Science Center, Ehime University*

17:20 - 17:40

1L11 Management of cell samples in in-cell NMR spectroscopy

○Kohsuke Inomata¹, Mei Toyoda¹, Kaito Shima¹, Moeka Nagamine¹, Shiori Suehiro¹, Teppei Ikeya¹, Takafumi Suzuki², Masayuki Yamamoto^{2,3}, Yutaka Ito¹
1 *Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University*
2 *Department of Medical Biochemistry, Tohoku University Graduate School of medicine*
3 *Tohoku Medical Megabank Organization, Tohoku University*

17:40 - 18:00

1L12 In-cell NMR study on the interaction of HIV Tat-binding RNA aptamer with its target molecule in living human cells

○Yudai Yamaoki^{1,2}, Omar Eladl^{1,2}, Keiko Kondo¹, Takashi Nagata^{1,2}, Masato Katahira^{1,2}
1 *Institute of Advanced Energy, Kyoto University*
2 *Graduate School of Energy Science, Kyoto University*

18:20 - 20:00 Board and Council Meeting [venue: Sangyo-Koryu Plaza 1st Room]

Day 2 (Wed. 8th Nov.)

9:30 - 17:00 Poter Exhibition 【venue: Small Hall 5F】

9:30 - 18:00 Corporate Exhibition 【venue: Large Hall Foyer 4F & Small Hall Entrance 4F】

Presentation IV [Large Hall]

9:30 - 10:10 Chairperson: Tomoyasu Aizawa

9:30 - 9:50

2L01 Secondary structures of 3' untranslated region controlling genome replication for SARSCoV-2

○Takako Ohyama^{1,2}, Takuo Osawa², Shun-ichi Sekine², and Yoshitaka Ishii^{1,2}

1 *School of Life Science and Technology, Tokyo Institute of Technology*

2 *Center for Biosystems Dynamics Research, RIKEN*

9:50 - 10:10

2L02 Dynamically regulated two-site interaction of viral RNA to capture host translation initiation factor

○Shunsuke Imai¹, Hiroshi Suzuki², Yoshinori Fujiyoshi², Ichio Shimada^{1,3}

1 *RIKEN Center for Biosystems Dynamics Research*

2 *Cellular and Structural Physiology Laboratory (CeSPL),
Tokyo Medical and Dental University*

3 *Graduate School of Integrated Sciences for Life, Hiroshima University*

Presentation V [Large Hall]

10:10 - 10:50 Chairperson: Yoh Matsuki

10:10 - 10:30

2L03 Quantitative solid-state, DNP-NMR analysis of amorphous structures and their applications to organic light-emitting diodes

○Hironori Kaji, Katsuaki Suzuki

Institute for Chemical Research, Kyoto University

10:30 - 10:50

2L04 Hyperpolarization of drug molecules in cocrystals at room temperature using photoexcited electrons

○Munehiro Inukai¹, Haruki Sato², Koichiro Miyamishi^{3,4}, Makoto Negoro^{4,5}, Akinori Kagawa⁶,
Koichi Nakamura¹

1 *Graduate School of Technology, Industrial and Social Sciences, University of Tokushima*

2 *Graduate School of Sciences and Technology for Innovation, University of Tokushima*

3 *Graduate School of Engineering Science, University of Osaka*

4 *Center for Quantum Information and Quantum Biology, University of Osaka*

5 *Institute for Quantum Life Science, National Institutes for Quantum Science and Technology*

6 *Premium Research Institute for Human Metaverse Medicine, University of Osaka*

10:50 - 11:05 Break Time

English Session 【venue: Large Hall】

Chairpersons: Yoshitaka Ishii, Chojiro Kojima

11:05 - 11:25 Chairperson: Yoshitaka Ishii

2L05 Chlorine-35/37, Bromine-79/81, and Iodine-127 NMR Spectroscopy of Organic Solids

○Kazuhiko Yamada

*Interdisciplinary Science Unit, Multidisciplinary Sciences Cluster,
Research and Education Faculty, Kochi University*

11:25 - 12:05 Chairperson: Chojiro Kojima

11:25 - 11:45

2L06 Residue-based correlation between equilibrium and rate constants is an experimental formulation of the consistency principle for smooth structural changes of proteins

○Daisuke Kohda¹, Seiichiro Hayashi¹, Daisuke Fujinami²

1 Medical Institute of Bioregulation, Kyushu University

*2 Graduate School of Integrated Pharmaceutical and Nutritional Sciences,
University of Shizuoka*

11:45 - 12:05

2L07 Effect of phosphorylation on structure, dynamics, and properties of N-terminal domain of spider dragline silk protein: implication on artificial spider dragline silk synthesis

○Nur Alia Oktaviani¹, Hamish C. Craig¹, Mami Goto¹, Fumiaki Hayashi², Keiji Numata^{1,3}

1 Biomacromolecules research team, RIKEN Center for Sustainable Resource Sciences

2 RIKEN Center for Biosystem Dynamics Research

3 Department of Material Chemistry, Graduate School of Engineering, Kyoto University

12:05 - 13:30 Lunch

Invited Lectures [venue: Large Hall]

13:30 - 15:15 Chairpersons: T. Ikegami (IL-1), A. Asano (IL-2), K. Takeda (IL-3)

13:30 - 14:05 Chairperson: Takahisa Ikegami

IL-1 Small molecules triggering transmembrane signaling and interfering with aggregation important in neurodegeneration studied by NMR

Xizhou Cecily Zhang¹, L. Antonschmidt¹, V. Sant¹, M. Han¹, M. Kim¹, B. Frieg², D. Matthes³, Siegfried Weisenburger⁴, K. Chakrabarty¹, S. Pratihari¹, D. Mukhopadhyay¹, A. Leonov¹, S. Ryazanov¹, A. Giese⁵, Vahid Sandoghdar⁴, G. Uden⁶, S. Becker¹, B. de Groot³, G. Schröder², L. B. Andreas¹, Christian Griesinger^{1,7}

1 NMR-based Structural Biology, Max-Planck-Institute for Multidisciplinary Sciences,

2 Institute of Biological Information Processing (IBI-7: Structural Biochemistry),

3 Department of Theoretical and Computational Biophysics, Max Planck Institute for Multidisciplinary Sciences,

4 Department Nano-Optics, Plasmonics and Biophotonics, Max Planck Institute for the Science of Light,

5 Center for Neuropathology and Prion Research, Ludwig-Maximilians-University Munich,

6 Institute for Microbiology and Wine Research, Johannes Gutenberg University of Mainz,

7 Cluster of Excellence "Multiscale Bioimaging: From Molecular Machines to Networks of Excitable Cells" (MBExC), University of Göttingen,

14:05 - 14:40 Chairperson: Atsushi Asano

IL-2 Characterizing polyamide reverse osmosis membranes via solid-state NMR methods

○Ryan C. Nieuwendaal

Materials Science and Engineering Division, National Institute of Standards and Technology

14:40 - 15:15 Chairperson: Kazuyuki Takeda

IL-3 Magnetic resonance in superconducting quantum computers

○Yutaka Tabuchi

RIKEN Center for Quantum Computing

15:15 - 15:35 Break Time

15:35 - 15:45 Award Ceremony by the NMRSJ
Chairperson: Koh Takeuchi, Yoh Matsuki

Award Lectures [venue: Large Hall]

15:45 - 16:35 Chairperson: Koh Takeuchi, Yoh Matsuki

15:45 - 16:10

AL-1 Characterization of retinal protonated Schiff base in microbial rhodopsin by solid-state NMR

○Izuru Kawamura

Graduate School of Engineering Science, Yokohama National University

16:10 - 16:35

AL-2 Function-related conformational dynamics of eukaryotic membrane proteins in lipid bilayers revealed by solution NMR with novel stable isotope labeling methods

○Yutaka Kofuku

Graduate School of Pharmaceutical Sciences, The University of Tokyo

16:35 - 16:45 Break Time (For preparation of Ceremony)

16:45 - 16:55 Honorary-Member Award Ceremony by the NMRSJ
Chairperson: Toshimichi Fujiwara, President of the NMRSJ

16:55 - 17:00 Break Time (For preparation of Lecture)

Honorary Lectures [venue: Large Hall]

17:00 - 18:10 Chairperson: Masato Katahira (HL01), Koichi Kato (HL02)

17:00 - 17:35

HL-1 Solution NMR for the characterization of synthetic polymers: SEC-NMR and DOSY

○Koichi Ute

Department of Applied Chemistry, Tokushima University

17:35 - 18:10

HL-2 Development of NMR spectroscopy and its application to biomolecular systems

○Toshimichi Fujiwara

Institute for Protein Research, Osaka University

18:10 - 18:15 Honorary Lecture Ceremony by the NMRSJ
Chairperson: Takanori Kigawa, Vice President of the NMRSJ

18:45 - 21:00 **Banquet** [venue: Mercure Hotel 5F Paris Hall]

Day 3 (Thu. 9th Nov.)

Presentation VI [Large Hall]

9:15 - 10:15 Chairperson: Izuru Kawamura

9:15 - 9:35

3L01 NMR analyses of the molecular recognition mechanism of anti-VEGF RNA aptamer

○Koh Takeuchi¹, Ichio Shimada²

1 *Graduate School of Pharmaceutical Sciences, The University of Tokyo*

2 *RIKEN Center for Biosystems Dynamics Research*

9:35 - 9:55

3L02 Inhibitory mechanism of transcription factor FOXO3a by 14-3-3ζ

Shota Enomoto¹, Tomoya Kuwayama¹, Shoichi Nakatsuka¹, Mariko Yokogawa¹, Kosaku Kawatsu¹, Risa Nakamura¹, Tomomi Kimura¹, Mikio Tanabe², Toshiya Senda², Jun Saito³, Hideyuki Saya³, ○Masanori Osawa¹

1 *Grad. Sch. Pharm. Sci., Keio Univ.*, 2 *IMSS, KEK*, 3 *Cancer Center, Fujita Health Univ.*

9:55 - 10:15

3L03 Real-time monitoring of enzyme-catalyzed modification of anti-influenza prodrug favipiravir by time-lapse ¹⁹F, ³¹P-NMR measurements

○Toshihiko Sugiki¹, Akihiro Ito², Yuko Hatanaka^{3,4}, Masaki Tsukamoto⁵, Tsuyoshi Murata⁶, Koichiro Miyanishi^{3,4}, Akinori Kagawa^{3,4,7}, Toshimichi Fujiwara^{1,4}, Masahiro Kitagawa^{3,4}, Yasushi Morita⁶, Makoto Negoro^{4,8}

1 *Institute for Protein Research, Osaka University*

2 *Graduate School of Science, Osaka University*

3 *Graduate School of Engineering Science, Osaka University*

4 *Center for Quantum Information and Quantum Biology (QIQB), Osaka University*

5 *Graduate School of Informatics, Nagoya University*

6 *Faculty of Engineering, Aichi Institute of Technology*

7 *Premium Research Institute for Human Metaverse Medicine (WPI-PRIME), Osaka University*

8 *Institute for Quantum Life Science, National Institute for Quantum and Radiological Science and Technology (QST)*

10:15 - 12:15 Poster Session I (odd number -xx, 3P-xx) [Small Hall]

12:15 - 13:00 Remove Poster

12:15 - 13:30 Lunch

Presentation VII [Large Hall]

13:30 - 14:30 Chairperson: ~~Yoshitaka Ishii~~ => changed to Yusuke Nishiyama

13:30 - 13:50

3L04 CO₂/CH₄ Separation Mechanism in a Metal–Organic Framework Investigated by Solid-State NMR

○Takuya Kurihara¹, Munehiro Inukai², Yusuke Nishiyama³, Motohiro Mizuno^{4,5}

1 *Graduate School of Natural Science and Technology, Kanazawa University*

2 *Graduate School of Technology, Industrial and Social Science, Tokushima University*

3 *JEOL Ltd.*

4 *Nanomaterials Research Institute, Kanazawa University*

5 *Institute for Frontier Science Initiative, Kanazawa University*

13:50 - 14:10

3L05 DNP enhanced ⁴³Ca and ¹⁷O NMR spectroscopy of cementitious materials

○Hiroki Nagashima¹, Akiko Sasaki¹, Koya Kamimura³, Chihiro Urata², Tsuyoshi Saito³

1 *Interdisciplinary Research Center for Catalytic Chemistry, AIST*

2 *Innovative Functional Materials Research Institute, AIST*

3 *Department of Civil Engineering, Niigata University*

14:10 - 14:30

3L06 Diffusion Constant Measurement for Ion Conductor Using Fringe Methods

○Miwa Murakami¹, Arunkumar Dorai¹, Nithya Hellar¹, Junichi Kawamura¹,
Takahisa Omata¹, Kiyonori Takegoshi²

1 *Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*

2 *Office of Society-Academia Collaboration for Innovation, Kyoto University*

14:30 - 14:45 Break Time

Presentation VIII [Large Hall]

14:45 - 15:45 Chairperson: Hideo Takahashi

14:45 - 15:05

3L07 Structural analysis by solution NMR reveals that multivalent interaction between multi-domain GRB2 and IDR SOS1-PR, and molecular mechanisms of LLPS

○Teppey Ikeya¹, Haruka Sugasawa¹, Naoyuki Togashi¹, Toshifumi Hayashi¹,
Tsutomu Mikawa^{1,2}, Yuji Sugita^{2,3}, Yutaka Ito¹

1 *Graduate School of Science, Tokyo Metropolitan University*

2 *Center for Biosystems Dynamics Research, RIKEN*

3 *Theoretical Molecular Science Laboratory, RIKEN Cluster for Pioneering Research, RIKEN*

15:05 - 15:25

3L08 Development of Stable Isotope Labeling Method in Eukaryotic Expression Systems

○Yutaka Kofuku¹, Taiga Yamamoto¹, Yutaro Ogaeri¹, Yuji Tokunaga¹, Takumi Ueda¹,
Ichio Shimada^{1,2}, Koh Takeuchi¹

1 Graduate School of Pharmaceutica Sciences, The University of Tokyo

2 RIKEN Center for Biosystems Dynamics Research

15:25 - 15:45

3L09 Identification of charge-neutral lysine sidechain

○Masaki Mishima

Department of Molecular Biophysics, School of Pharmacy,

Tokyo University of Pharmacy and Life Sciences

15:45 - 15:50

Closing Remarks