Program

TUESDAY, OCTOBER 4, 2016

15:00–17:00 Registration

17:10–17:15 Opening Remarks: Ichio SHIMADA

17:15–17:55 Plenary Lecture 1
Chair: Ichio SHIMADA

The role of solution NMR in 21st century structural biology ……**24**
Kurt WÜTHRICH
(Institute of Molecular Biology and Biophysics, ETH Zürich, Switzerland
The Scripps Research Institute, USA)

17:55–18:35 Plenary Lecture 2
Chair: Yoshinori FUJIYOSHI

Structural basis for channel activity of ryanodine receptor RyR1 ……**26**
Wayne A. HENDRICKSON
(Department of Biochemistry and Molecular Biophysics, Columbia University, USA/
Department of Physiology and Cellular Biophysics, Columbia University, USA)

18:40–20:30 Welcome Reception

WEDNESDAY, OCTOBER 5, 2016

9:00–12:30 Session A
Chairs: Ichio SHIMADA
Peter E. WRIGHT

9:00–9:30 **[A-1]**
Role of intrinsically disordered proteins in cellular signaling and regulation ……**28**
Peter E. WRIGHT
(The Scripps Research Institute, Department of Integrative Structural and Computational Biology, USA)

9:30–10:00 **[A-2]**
Cellular structural biology: from structures to functional processes ……**30**
Lucia BANCI
(University of Florence, CERM, Italy)

10:00–10:30 [A-3]

Structure and dynamics of HIV-1 capsid assemblies: insights from an integrated MAS NMR, MD simulations, and density functional theory approach ……**34**

Tatyana POLENOVA

(Department of Chemistry and Biochemistry, University of Delaware, USA/ Pittsburgh Center for HIV Protein Interactions, University of Pittsburgh School of Medicine, Pittsburgh, USA)

10:30–11:00 Coffee Break

11:00–11:30 [A-4]

***In situ* structural biology by NMR** ……**36**

Yutaka ITO

(Department of Chemistry, Tokyo Metropolitan University, Japan/ CREST, Japan Science and Technology Agancy, Japan)

11:30–12:00 [A-5]

Advanced stable-isotope labeling strategies for biomolecular NMR spectroscopy ……**38**

Takanori KIGAWA

(RIKEN Quantitative Biology Center (QBiC), Japan/ Department of Computer Science, School of Computing, Tokyo Institute of Technology, Japan)

12:00–12:15 [A-6 (PS NO. 11)]

Advanced instrumentation for DNP–enhanced MAS NMR for higher magnetic fields and lower temperatures ……**99**

Yoh MATSUKI

(Institute for Protein Research, Osaka University, Japan)

12:15–12:30 [A-7 (PS NO. 21)]

High pressure NMR reveals a fluctuating ubiquitin structure ……**109**

Ryo KITAHARA

(College of Pharmaceutical Sciences, Ritsumeikan University, Japan)

12:30–14:00 Lunch

14:00–17:30 Session B

Chairs: Osamu NUREKI
Nieng YAN

14:00–14:30 [B-1]

Structural physiology of channels ……**42**

Yoshinori FUJIYOSHI

(Graduate School of Pharmaceutical Sciences, Nagoya University/ CeSPI, Japan)

14:30–15:00 [B-2]

Single particle cryo-EM of integral membrane proteins at crystallographic resolution ……**44**

Yifan CHENG

(HHMI/Department of Biochemistry and Biophysics, University of California San Francisco, USA)

15:00–15:30 [B-3]
Structural and mechanistic investigation of the human glucose transporters GLUTs ·····48
Nieng YAN
(Tsinghua University School of Medicine, China)

15:30–16:00 Coffee Break

16:00–16:30 [B-4]
Membrane protein structures and Free Electron Laser ·····50
So IWATA
(Graduate School of Medicine Kyoto University, RIKEN SPring-8 Center, Japan)

16:30–17:00 [B-5]
Mechanism of photosynthetic water oxidation based on atomic structure of photosystem II ·····52
Jian-Ren SHEN
(Research Institute for Interdisciplinary Science, Okayama University, Japan/
Institute of Botany, Chinese Academy of Sciences, Beijing, China)

17:00–17:15 [B-6 (PS NO. 27)]
Snapshots of a proton−driven protein translocation motor ·····115
Tomoya TSUKAZAKI
(Graduate School of Biological Sciences, Nara Institute of Science and Technology, Japan)

17:15–17:30 [B-7 (PS NO. 55)]
Structural mechanisms of receptor−mediated selective autophagy of aggregated aminopeptidase ·····145
Nobuo N. NODA
(Institute of Microbial Chemistry, Microbial Chemistry Research Foundation, Japan)

17:30–19:30 Dinner

19:30–21:30 Poster Session [I] Odd Numbers

THURSDAY, OCTOBER 6, 2016

9:00–12:30 Session C
Chairs: Hidehito TOCHIO
Angela M. GRONENBORN

9:00–9:30 [C-1]
Structural study of proinflammatory cytokine IL-18 ·····54
Hidehito TOCHIO
(Department of Biophysics, Graduate School of Science, Kyoto University, Japan)

9:30–10:00 [C-2]

Multidrug recognition and transcriptional regulation of a multidrug transcriptional repressor LmrR ·····56

Koh TAKEUCHI

(Molecular Profiling Research Center, National Institute of Advanced Industrial Science and Technology, Japan/ PRESTO, Japan science and technology agency, Japan)

10:00–10:30 [C-3]

Molecular chaperones in action ·····58

Charalampos Babis KALODIMOS

(Department of Biochemistry, Biophysics and Molecular Biology, University of Minnesota, USA)

10:30–11:00 Coffee Break

11:00–11:30 [C-4]

Structural basis for dynamic orchestration of proteasomes ·····60

Koichi KATO

(Department of Bioorganization Research, Okazaki Institute for Integrative Bioscience and Institute for Molecular Science, National Institutes of Natural Sciences, Japan/ Department of Structural Biology and Biomolecular Engineering, Graduate School of Pharmaceutical Sciences, Nagoya City University, Japan)

11:30–12:00 [C-5]

Synergy between NMR, Cryo-EM and large-scale MD simulations—an all atom model of a native HIV capsid ·····62

Angela M. GRONENBORN

(Department of Structural Biology, University of Pittsburgh School of Medicine, USA)

12:00–12:15 [C-6 (PS NO. 2)]

Structural basis for the inhibition of voltage-dependent K^+ channel by gating modifier toxin ·····88

Masanori OSAWA

(Keio University Faculty of Pharmacy, Japan)

12:15–12:30 [C-7 (PS NO. 20)]

Structural basis for the regulation of enzymatic activity of Regnase-1 by domain-domain interactions ·····108

Mariko YOKOGAWA

(Faculty of Advanced Life Science, Hokkaido University, Japan)

12:30–14:00 Lunch

14:00–17:30 Session D

Chairs: Toshiyuki SHIMIZU
Simon NEWSTEAD

14:00–14:30 [D-1]

Crossing the barrier: Towards a molecular understanding of proton coupled peptide uptake via the PTR/NRT family of membrane transporters ·····64

Simon NEWSTEAD

(University of Oxford, UK)

14:30–15:00 [D-2]

Structures and molecular mechanisms of membrane transporters ……66

Osamu NUREKI
(Department of Biological Sciences, Graduate School of Science, The University of Tokyo, Japan)

15:00–15:30 [D-3]

Structural studies of cytochrome c oxidase functioning in the mitochondrial inner-membrane ……68

Tomitake TSUKIHARA
(Department of Life Science, University of Hyogo, Japan/ Institute for Protein Research, Osaka University, Japan)

15:30–16:00 Coffee Break

16:00–16:30 [D-4]

Innate immune mechanism for viral dsRNA recognition ……70

Sun HUR
(Harvard Medical School, USA)

16:30–17:00 [D-5]

Structural study of TLRs sensing single stranded RNA in innate immune system ……72

Toshiyuki SHIMIZU
(Graduate School of Pharmaceutical Sciences, The University of Tokyo, Japan)

17:00–17:15 [D-6 (PS NO. 24)]

Crystal structure of NOD2 reveals its implications in human diseases ……112

Umeharu OHTO
(Graduate School of Pharmaceutical Sciences, The University of Tokyo, Japan)

17:15–17:30 [D-7 (PS NO. 34)]

RNA-guided DNA cleavage mechanism of class 2 CRISPR-Cas effectors ……123

Hiroshi NISHIMASU
(Department of Biological Sciences, Graduate School of Science, The University of Tokyo, Japan)

17:30–19:30 Dinner

19:30–21:30 Poster Session [II]:Even Numbers

FRIDAY, OCTOBER 7, 2016

9:00–12:00 Session E
Chair: Kurt WÜTHRICH

9:00–9:10 **[E-1]**

Kurt WÜTHRICH
(Institute of Molecular Biology and Biophysics, ETH Zurich, Switzerland
The Scripps Research Institute, USA)

9:10–9:45 **[E-2]**
NMR Approaches to Dissect Oncogenic RAS Signaling At Biological Membrane Interface ····74
Mitsu IKURA
(Princess Margaret Cancer Centre, University of Toronto, Canada)

9:45–10:20 **[E-3]**
Integrative structural biology approach to decipher the molecular mechanism of Asn-glycosylation ····76
Daisuke KOHDA
(Medical Institute of Bioregulation, Kyushu University, Japan)

10:20–10:50 Coffee Break

10:50–11:25 **[E-4]**
Functional equilibrium of membrane proteins ····80
Ichio SHIMADA
(Graduate School of Pharmaceutical Sciences,
The University of Tokyo, Japan)

11:25–12:00 **[E-5]**
***Large-amplitude, slow breathing motions* in proteins as evaluated by aromatic ring flipping motions–Insights into the dynamics of protein interiors and protein–ligand interfaces** ····82
Masatsune KAINOSHO
(Graduate School of Science and Engineering,
Tokyo Metropolitan University, Japan)

12:00–12:10 Announcement of Grant Recipients

12:10–12:15 Closing Remarks: Toshiyuki SHIMIZU

12:15–13:00 Lunch