

## Poster Titles submitted to ISDSB2016

発表総数 30 の内 6 件 (#1, #4, #5, #10, #14, #23) が日本からの参加者によるもの

- 1) An effective deuterium exchange method for a neutron structure analysis by use of unfolding-refolding processes. Akiko Kita and Yukio Morimoto (Research Reactor Institute, Kyoto University).
- 2) Flanking Mismatches Alter the Structure and Function of the APE1/DNA Complex. AM Whitaker, MS Fairlamb and BD Freudenthal.
- 3) Developing semi-synthetic composite materials for investigating cellulose and matrix polymer interactions during pretreatment. Riddhi Shah, Hugh O'Neill, Daisuke Sawada, Sai Venkatesh Pingali, Loukas Petridis, Volker Urban, Paul Langan, Arthur J. Ragauskas, Jeremy C Smith.
- 4) TRAIL-R 2 Superoligomerization Induced by Human Monoclonal Agonistic Antibody KMTR2. Taro Tamada, Daisuke Shinmi, Masahiro Ikeda, Eiji Mori, Kazuhiro Motoki.
- 5) High-resolution crystal structures of the hemi-binding domain of porcine cytochrome b<sub>5</sub>. Yu Hirano, Shigenobu Kimura, Taro Tamada, Tokai Quant. Beam Sci. Cent., QST <sup>2</sup>Fac. Of Engin, Ibaraki Univ.
- 6) Structural determination of DNA polymerase complex from Nanoarchaeum equitans using segmental labelling and small-angle scattering techniques. Qiu Zhang, Ryan C, Oliver, Sai Venkatesh Pingali, Leighton Coates, Hugh O'Neill, and Volker Urban.
- 7) Understanding Trichoderma reesi Cel7A Mechanism of Cellulose Depolymerization Through Crystallography. Annette Bodenheimer, Flora Meilleur.
- 8) Joint X-ray/Neutron Structures of the Helicobacter pylori 5'-methylthioadenosine Nucleosidase Describe Proton Sharing and Protonation States. Michael T. Banco, Vidhi Mishra, Andreas Ostermann, Tobias E. Schrader, Gary B. Evans, Andrey Y. Kovalevsky, and Donald R. Ronning.
- 9) DFT/MM Simulations of the L-arabinose-Xylose Isonerose Complex with Mg<sup>2+</sup> and Cd<sup>2+</sup>. Troy Wymore, Jerry M. Parks, Jeremy C. Smith, Paul Langan, and Andrey Kovalevsky.
- 10) Neutron diffractometer for protein crystallography covering crystals with large unit cell volume at J-PARC. Kazuo Kurihara, Katsuaki Tomoyori, Yu Hirano, Taro Tamada.

- 11) SANS Study of Moisture-Induced Changes in Chemically Treated Wood Cell Walls. Nayomi Plaza, Charles Frihart, Dan Yelle, Chris Hunt, Don Stone, Sai Venkatesh Pingali, Joseph E. Jakes.
- 12) Tension wood provides insight into structural changes in biomass resulting from chemical pretreatment. Sai Venkatesh Pingali, Daisuke Sawada, Udaya Kalluri, Hugh O'Neill, Volker Urban, Paul Langan, and Brian H. Davison.
- 13) Highly resistant HIV-1 proteases and strategies for their inhibition. Andres Wong-Sam, Daniel W. Kneller, and Irene T. Weber.
- 14) Application of profile fitting method to neutron time-of-flight protein single crystal diffraction data collected at the IBI. Naomine Yano, Taro Yamada, Takaaki Hosoya, Takashi Ohhara, Ichiro Tanaka, Katsuhiko Kusaka.
- 15) New Capabilities at the Oak Ridge National Lab Center for Structural Molecular Biology. Ryan C. Oliver, Volker Urban, Sai Venkatesh Pingali, Shuo Qian, Hugh O'Neill, Kevin L. Weiss, Qiu Zhang, Paul Langan.
- 16) Visualizing the Bohr effect in hemoglobin: neutron structure of equine cyanomet-hemoglobin in the R-state and comparison with human deoxy-hemoglobin in the T-state. Steven Dajnowicz, Sean Seaver, Leif Hanson, S. Zoe Fisher, Paul Langan, Andrey Kovalevsky, Timothy Mueser.
- 17) A Structural, Computational, and Inhibitory Study of *Mycobacterium tuberculosis* Ag85C Covalently Modified by Ebselen Derivatives. Christopher M. Goins, Sandeep Thanna, Steven Dajnowicz, Steven J. Sucheck, Donald R. Ronning.
- 18) Inhibitor development against aspartate semialdehyde dehydrogenase: X-ray crystallography, docking and molecular dynamics approaches. Gopal P. Dahal and Ronald E. Viola.
- 19) GlgE: the addition of maltose to an  $\alpha$ -glucan through an  $S_N1$  mechanism. Cecile Petit, Jared Lindenberger, Sandeep Thanna, Sri Kamar Veleti, Steven J. Sucheck, and Donald Ronning.
- 20) Mutation of putative nucleophile Glu303 has a differential effect on kinetics and structure of the human ABO(H) blood group glycosyltransferases GTA and GTB. Susannah M.L. Gagnon, Ryan J. Blacker, Robert Polakowski, Natisha Rose, Ruixiang Zheng, James A. Letts, Asha Johal, Brock Schuman, Svetlana N. Borisova, Monica M. Palcic, Stephen V. Evans.

- 21) Increasing terpene content in foliage of Eucalyptus for specialty biofuels. Aparna Annamraju, Durgesh K. Rai, Ritesh Mewalal, Lee E Gunter, Paul E Abraham, Sai Venkatesh Pingali, Hugh O'Neill, Nancy L Engle, Timothy J Tschplanski and Gerald A Tuskan.
- 22) *In-Vivo* Probing Lateral Organization of Lipid Membranes using SANS. S. Chatterjee, J. Nickels, J. Katsaras, R. F. Standaert, D. A. A. Myles, and J. G. Elkins.
- 23) Analysis of the Catalytic Mechanism of Copper Amine Oxidase from *Arthrobacter Globiformis*. Hiroshi Yamaguchi, Takeshi Murakawa, Misumi Kataoka, Yoshiaki Kawano, Hideyuki Hayashi, Katsuyuki Tanizawa, and Toshihide Okajima.
- 24) Neutron Crystallographic Studies of HIV-1 Protease: Drug Binding, Drug Resistance, and Proton Transfer. Andrey Kovalevsky, Oksana Gerlits, Troy Wymore, Amit Das, Chen-Hsian Shen, Jerry M. Parks, Jeremy C. Smith, Kevin Weiss, David A. Keen, Matthew P. Blakeley, John M. Louis, Paul Langan, and Irene Weber.
- 25) Neutron Diffraction Studies of a HAD Superfamily Model Enzyme, KDN9DD. Katherine H. O'Toole, Tyrel Bryan, Daniel Saltzberg, Andrey Kovalevsky, Debra Dunaway-Mariano, Karen N. Allen.
- 26) Making an Aquaporin Water-tight: The Structural Basis of Selectivity of Plant Nodulin 26-Intrinsic Proteins. Zach Beamer, Tian Li, Andrey Kovalevsky, and Daniel M. Roberts.
- 27) Crystallographic Studies of Human Acetylcholinesterase Reactivation by Oximes. Oksana Gerlits, Mikolai Fajer, Xiaolin Cheng, Donald Blumenthal, Palmer Taylor, Zoran Radic, and Andrey Kovalevsky.
- 28) Protonation States and pK<sub>a</sub>s in Xylanase II, Combining Neutron Crystallography and Molecular Simulation. Jerry M. Parks, Qun Wan, B. Leif Hanson, Suzanne Zoe Fisher, Andreas Ostermann, Tobias E. Schrader, David E. Graham, Leighton Coates, Paul Langan, and Andrey Kovalevsky.
- 29) Structural and Dynamical Insights into Substrate Recognition by Maltose-binding Proteins in *Thermotoga Maritima*. Shantanu Shukla, Caeley A. Gullett, Khushboo Bafna, Pratul K. Agarwal, Dean A. A. Myles, and Mathew J. Cuneo.
- 30) Investigating the Multiple Functions of Dehaloperoxidase Through Ligand Binding and H-bonding Networks: An X-ray and Neutron Crystallographic Study. Leiah M. Carey, Flora Meilleur, Dean A. A. Myles, Reza A. Ghiladi.