

**IUCr2008 Osaka Satellite Meeting**  
**Symposium on Neutron Protein Crystallography (NPC)**

- Current Status and Future Prospect -

*August 21-22, 2008*  
*Multi-purpose Hall, Ricotti in Tokai, Ibaraki Prefecture*

**Organized by**

Frontier Research Center for Applied Atomic Sciences, Ibaraki University  
Quantum Beam Science Directorate, Japan Atomic Energy Agency

The 169th Committee on Diffraction Structural Biology of  
University-Industry Cooperative Research Committee of Japan Society  
for the Promotion of Science (JSPS)

**Aug 21<sup>st</sup> (Thursday)**

Registration (9:00 - 10:00) (Entrance of the Hall)

Opening Remark (10:00 - 10:05) **Niimura, Nobuo** (Ibaraki University, Japan)

Morning Session (10:05 - 12:15) - Facility report -

*Chairperson: Niimura, Nobuo. (Ibaraki University, Japan)*

10:05 - 10:35 **Kurihara, Kazuo** (Japan Atomic Energy Agency, Japan)

"Recent Data Collections Using Neutron single-crystal diffractometers dedicated for biological macromolecules at JAEA"

10:35 - 11:05 **Tanaka, Ichiro** (Ibaraki University, Japan)

"Outline of a New Biological Neutron Diffractometer (iBIX) in J-PARC"

11:05 - 11:35 **Blakeley, Matthew** (Institut Laue Langevin, France)

"Neutron Macromolecular Crystallography using LADI-III"

11:35 - 12:05 **Coates, Leighton** (Oak Ridge National Laboratory, U.S.A.)

"The Macromolecular Neutron Diffractometer (MaNDi) under construction at the Spallation Neutron Source"

12:05 - 12:15 (**Not yet decided**)

"LANSCE, PCS - Brief comment -"

Lunch (12:15 - 13:30)

Afternoon session (13:30 - 15:45) - Neutron Protein Crystallography (1) / Invited talks -

*Chairperson: Tanaka, Ichiro. (Ibaraki University, Japan)*

13:30 - 14:15 **Glusker, Jenney** (Los Alamos National Laboratory, U.S.A.)

"Time-of-flight neutron structure of D-xylose isomerase"

14:15 - 15:00 **Chatake, Toshiyuki** (Kyoto University, Japan)

"Time of Flight Neutron Crystallographic Analysis of Human Deoxyhemoglobin"

15:00 - 15:45 **Blum, Marc-Michael** (Blum - Scientific Services, Germany) and **Chen, Julian** (Goethe University Frankfurt, Germany)

**"Application of Joint Neutron and X-ray Diffraction Refinement for Rapid Determination of Hydrogen Positions, Solvent Structure and Protonation States in Diisopropyl fluorophosphatase (DFPase)"**

Photo (15:45 - 16:00) (Hall)

Poster session (16:00 - 18:00) (Lounge)

Banquet (18:30 - 20:00) (Meeting room No.1 and No.2 (3F))

## **Aug 22<sup>nd</sup> (Friday)**

Morning Session (9:30 - 12:15) - Neutron Protein Crystallography (2) / Contributed talks -

*Chairperson: Podjarny, Alberto (Institut de Génétique et de Biologie Moléculaire et Cellulaire, France)*

9:30 - 10:00 **Yamada, Taro** (Ibaraki University, Japan)

**"A Neutron Crystallographic Analysis of a "phosphate-free" Ribonuclease A at 1.4 Å Resolution"**

10:00 - 10:30 **Ohnishi, Yuki** (Ibaraki University, Japan)

**"Large single crystal growth and preliminary neutron diffraction analysis of *Achromobacter protease I*"**

10:30 - 11:00 **Oksanen, Esko** (University of Helsinki, Finland)

**"Yeast Pyrophosphatase – towards a neutron structure"**

Break (11:00 - 11:15) (Meeting room No.3 (1F))

11:15 - 11:45 **Kuroki, Ryota** (Japan Atomic Energy Agency, Japan)

**"Inhibitor Recognition through Low Barrier Hydrogen Bonds and Oxianion Hole in Porcine Pancreatic Elastase Revealed by Neutron Crystallography"**

11:45 - 12:15 **Adachi, Motoyasu** (Japan Atomic Energy Agency, Japan)

**"Neutron Crystallography for Investigation of Catalytic Mechanism of Enzymes"**

Lunch (12:15 - 13:30)

Afternoon Session (13:30 - 15:00) - Neutron Protein Crystallography (3) / Invited talks -

*Chairperson: Kuroki, Ryota (JAERI, Japan)*

13:30 - 14:15 **Mitchler, Andre** (Institut de Génétique et de Biologie Moléculaire et Cellulaire, France)

**"Full deuteration of protein allows Neutron Laue diffraction with a single crystal volume significantly less than 1 mm<sup>3</sup>"**

14:15 - 15:00 **Kamikubo, Hironari** (Nara Institute of Science and Technology, Japan)

**"Direct observation of two distinct types of short hydrogen bond in Photoactive Yellow Protein"**

Closing Remark (15:00 - 15:05) **Kuroki, Ryota** (JAERI, Japan)

J-PARC Tour (15:30 - 17:25)

15:30	Bus departs from Ricotti
15:45- 17:10	J-PARC Tour
17:15	Bus stops at Akogi-ga-ura club
17:25	Bus arrives at Tokai Station