



◆◆◆ 27 January (Wed.) 9:30~17:00 ◆◆◆

— (K.Takano (Osaka Univ.)) —

- 9:30-10:00 「Protein crystallization for a large single crystal based on phase diagram (tentative)」  
Y. Ohnishi (Ibaraki Univ.)
- 10:00-10:30 「Protein Crystallization by Solution Flow Control」  
H. Matsumura (Osaka Univ.)
- 10:30-11:00 「Neutron protein crystallography in Ibaraki University (tentative)」  
T. Yamada (Ibaraki Univ.)
- 11:00-11:20 「Hydration structure around nucleotides」  
Y. Sugawara (Kitasato Univ.)

oo

11:20-12:15 Lunch (Lunch Box will be distributed.)

oo

—(N.Niimura)—

- 12:15-13:15 「Versatile or nasty, but clearly ubiquitous: Water as a partner in protein-ligand interactions」  
Gerhard Klebe (Philipps-Univ. Marburg)
- 13:15-13:45 「Hydration analysis of polyelectrolytes and proteins under enzyme reaction by dielectric relaxation spectroscopy.」  
M. Suzuki (Tohoku Univ.)

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13:45-14:00 Coffee Break (15 min)

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*(I. Tanaka) (Ibaraki U.)*

- 14:00-14:30 「Empirical distribution function of hydration water molecules around polar protein atoms and the application to predict hydration structures of proteins」  
D. Matsuoka, M. Nakasako (Keio Univ.)
- 14:30-15:00 「Hydration of Biomacromolecules: Protein and DNA」  
T. Chatake (Kyoto Univ.)
- 15:00-15:30 Discussion and summary (S.Ikemizu, K.Chiba, M.Sakurai, *C.Sasaki*)
- 16:00-17:00 J-PARC tour

◆◆◆ 28 January (Thu.) 9:30~12:30 ◆◆◆

**Workshop**  
**on**  
**Neutron & Hydration**  
**(Tentative)**

**Date: 28 January 2010 9:30-12:30**

**Place: IQBRC D311 (Tentative)**

9:30-9:40 Introductory Talk (N.Niimura)

9:40-10:25 Versatile or nasty, but clearly ubiquitous: Water as a partner in protein-ligand interactions (Part II) (G. Klebe)

10:25-10:35 Comments on hydration in proteins (M.Suzuki)

10:35-10:45 Thrombin – ligand interaction (T.Yamada)

10:45-10:55 Trypsin – BPTI interaction (K.Kawamura)

10:55-11:05 API –catalytic triad (Y. Ohnishi)

11:05-11:15 (M.Unno)

11:15-12:30 Discussion on neutron & hydration (All participants)