國立清華大學
生命科學院
NATIONAL TSING HUA UNIVERSITY
COLLEGE OF LIFE SCIENCE

Special Seminar

Title：**Computational design of selective ion-binding proteins**

Speaker：**Dr. Sakuraba Shun**
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Time：10:00, Monday, March 3, 2014

Place：Room 105 , LS Building II

Host：楊立威老師 Prof. Lee-Wei Yang

Language：English

※歡迎聽講※

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Modern structural biology, combined with computer modeling and simulations, enabled the rational design of drug molecules that specifically binds to the target protein.
Is it possible to do that in reverse? Can we design protein amino acid sequence that specifically binds to a single molecule?
In this talk, as the simplest example of such problems, I will explain my ongoing research project about the design of ion-binding protein.
With a combination of discrete optimization and molecular dynamics simulations, we redesigned 115-residues protein that selectively binds to the caesium ion.
Algorithms and the structural insights are discussed.

Dr Sakuraba Shun
Full Publication List (peer-reviewed)
1. Adaptive Lambda Square Dynamics Simulation: an E_cient Conformational Sampling Method for Biomolecules.
Jinzen Ikebe, Shun Sakuraba, Hidetoshi Kono, J. Comp. Chem., 35, 39_50 (2014).
2. Free-energy Analysis of Lysozyme-triNAG Binding Modes With All-atom Molecular Dynamics Simulation Combined With the Solution Theory in the Energy Representation.
Kazuhiro Takemura, Raghunadha Reddy Burri, Takeshi Ishikawa, Takakazu Ishikura, Shun Sakuraba, Nobuyuki Matubayasi, Kazuo Kuwata, Akio Kitao, Chem. Phys. Lett., 559, 94_98.
3. Evaluation of Protein-protein Docking Model Structures Using All-atom Molecular Dynamics Simulations Combined With the Solution Theory in the Energy Representation.
Kazuhiro Takemura, Hao Guo, Shun Sakuraba, Nobuyuki Matubayasi, and Akio Kitao, J. Chem. Phys., 137, 215105 (2012).
4. Interaction of Naphthalene Derivatives with Lipid in Membrane Studied by 1H-Nuclear Overhauser E_ect and Molecular Dynamics Simulation.
Megumi Shintani, Yushi Matsuo, Shun Sakuraba, Nobuyuki Matubayasi, Phys. Chem. Chem. Phys., 14, 14049 (2012).
5. Distribution-Function Approach to Free-Energy Computation.

Shun Sakuraba and Nobuyuki Matubayasi, J. Chem. Phys., 135, 114108 (2011).

6. NMR-NOE and MD Simulation Study on Phospholipid Membranes: Dependence on Membrane Diameter and Multiple Time Scale Dynamics.
Megumi Shintani, Ken Yoshida, Shun Sakuraba, Masaru Nakahara, and Nobuyuki Matubayasi, J. Phys. Chem. B 115, 9106_9115 (2011).

7. Detecting Coupled Collective Motions in Protein by Independent Subspace Analysis.
Shun Sakuraba, Yasumasa Joti, and Akio Kitao, J. Chem. Phys. 133, 185102 (2010).

8. Multiple Markov Transition Matrix Method: Obtaining the Stationary Probability Distribution From Multiple Simulations.
Shun Sakuraba and Akio Kitao, J. Comput. Chem. 30, 1850_1858 (2009).

9. Short Synthesis of (+)-Cylindricine C by Using a Catalytic Asymmetric Michael Reaction with a Two-Center Organocatalyst.
Tomoyuki Shibuguchi, Hisashi Mihara, Akiyoshi Kuramochi, Shun Sakuraba, Takashi Ohshima, and Masakatsu Shibasaki, Angew. Chemie 45, 4635_4637 (2006).