Asia Pacific Protein Association

APPA2014 Jeju

The 4th Asia Pacific Protein Association (APPA) Conference

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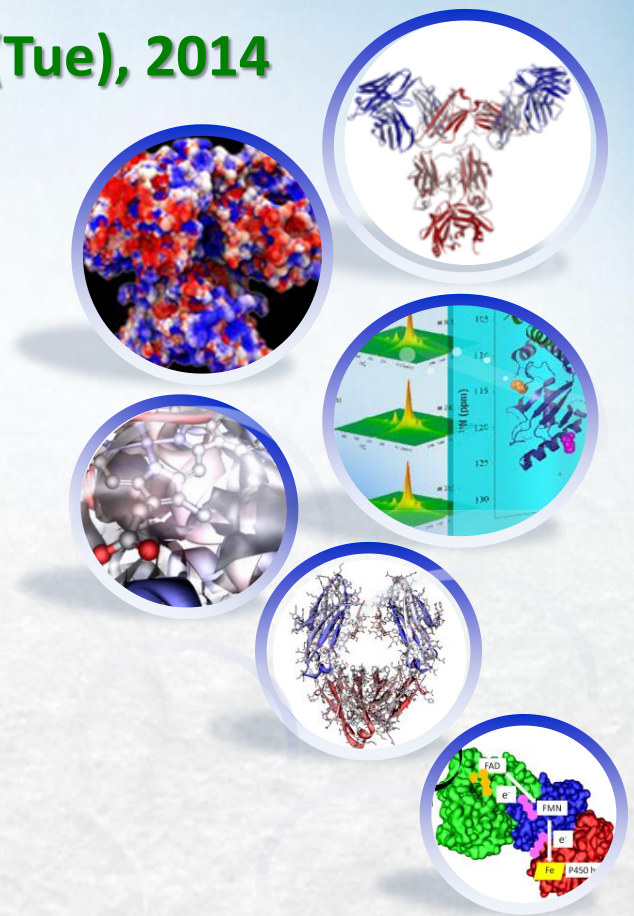
Place : ICC Jeju, Korea



Program & Abstracts

Organizer: Asia Pacific Protein Association
The Protein Society

Host: Korean Society for Protein Science
Korean Magnetic Resonance Society

Plenary Lectures II

New Approach to Electrostatic Properties of Proteins and Protein-Protein Interactions
May 18 (Sun), 11:30-12:10, ROOM: YEONGJU A
Chair: Kyou-Hoon Han, Ph.D. (APPA2014 co-chair & KSPS president, Korea)

Haruki Nakamura, Ph.D.
Institute for Protein Research, Osaka University, Japan

Professor Nakamura obtained his Ph.D. from University of Tokyo, Japan. His research fields include biophysics, protein science, and structural bioinformatics. From 2012, he is the Advisor to Osaka University Trustees.

Haruki Nakamura is a Professor of Laboratory of Protein Informatics, Institute for Protein Research, Osaka University. He is also a Head of Protein Data Bank Japan (PDBj, http://pdbj.org/), one of the four members of the wwPDB (http://wwpdb.org/) as the international organization to look after PDB. He was born on 7 April 1952, at Tokyo, Japan. He graduated Department of Physics, Faculty of Science, the University of Tokyo, in March 1975, and he took the Doctor of Science in March 1980, at Department of Physics, Faculty of Science, The University of Tokyo, supervised by Dr. Akiyoshi Wada.

His research experiences are as follows: April 1980 - July 1987, Research Associate at Department of Applied Physics, Faculty of Engineering, the University of Tokyo. August 1987 - March 1996, Protein Engineering Research Institute, Osaka. April 1996 - March 1999, Biomolecular Engineering Research Institute, Osaka. April 1999 -, Professor, Laboratory of Protein Informatics, Institute for Protein Research, Osaka University. April 2012 -, Advisor to Osaka University Trustees. June 2001 -, Head of PDBj.

His research fields are structural bioinformatics, biophysical studies about protein architecture, electrostatic properties and enzymatic functions, protein modeling, protein design, structure guided drug development, and molecular and electronic simulation. He is an associate Editor of BREV (Biophysical Reviews), and an editorial board member of PEDS (Protein Engineering Design and Selection), J. Struct. Funct. Genomics, and Biophysics.

Since 2012, he has been a Council member of the Protein Society until December 2014, and a President of Protein Science Society of Japan until March 2014. He is also a Council member of APPA.

Plenary Lecture II
May 18 (Sun), 11:30-12:10, ROOM: YEONGJU A

New Approach to Electrostatic Properties of Proteins and Protein-Protein Interactions

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Electrostatic properties of proteins govern most of the biological phenomena, in particular, specific molecular recognitions on protein interfaces, which controls biological signal transductions through protein-protein interactions (PPIs) [1-3]. Appropriate treatment of the electrostatic interaction is critical for computational analyses of PPI in a realistic manner. Since the potential function is long-range, it is not simple to handle the interactions in an effective manner: high accuracy, low computational cost, ease of the implementation, and freedom from artifacts. We have recently developed a novel algorithm, zero-multipole summation method, for evaluating the electrostatic energy of charged particle systems [4-6]. Its simple pair wise form enables us to effectively apply the scheme to high-performance parallel computation with GPGPU systems [7]. Several applications to homogeneous and inhomogeneous molecular systems have confirmed that it could replace the conventional Ewald method in order to perform rapid and accurate molecular dynamics simulations [8-10]. This method is applied to simulate a protein-protein docking procedure in an *ab-initio* manner, based on the computed free energy landscape [11, 12].

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