

# 信頼できる実験データと構造情報を得るために

From reliable experimental data to reliable structural data

## ▶ Abstract

March 2nd, 2024

AP Nihonbashi(Tokyo)



Wladek Minor

The University of Virginia

### Can structural biology keep pace with the digital revolution?

In this presentation, I will analyze several aspects of structural biology research, including its impact on other areas of science and recent developments that are transforming structural biology from mainly descriptive science into a digital one. The trends in structural biology revealed in this presentation provide crucial insights, particularly valuable in addressing emerging and recurring biomedical challenges and threats.



Yusuke Yamada

High Energy Accelerator  
Research Organization

### Automation and data management for macromolecular crystallography experiments at KEK Structural Biology Research Center

A large number of crystallization trials, data collection and structure determinations are necessary to make a structural biology research project successful, and automation of these experiments as well as management of resulting data are quite important.



Miki Senda\*, Toshiya Senda

High Energy Accelerator  
Research Organization

### A comprehensive strategy for quick determination of protein structures by MR-native SAD method

To achieve rapid structure determination, we need to overcome two bottlenecks: crystallization and phasing. Here, we present our crystallization techniques and the MR-native SAD method with low-energy X-ray.



Koh Takeuchi

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The University of Tokyo

## Connecting structures to function by NMR.

The function of macromolecules often depends on multiple conformational states. Thus, both reliable substate structures and their thermodynamic landscape would be required to describe macromolecules in action. NMR is a strong and complementary technique to advance and validate this scientific process by quantitative analyses of protein structure and dynamics in physiological conditions, both before and after high-resolution structures were solved.



Tadashi Satoh

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AgroDesign Studios

## Agrochemical SBDD based on massive structural data

Unlike pharmaceuticals, agrochemicals need to be effective against a broad range of organisms in the environment. Therefore, agrochemical SBDD requires massive structural data. In this symposium, we will present examples of novel herbicide discovery through this approach.



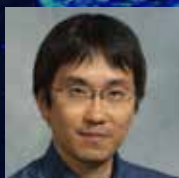
Raymond Burton-Smith

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National Institute  
for Physiological Sciences(NIPS)

## Balancing the demands of large subjects in cryo-electron microscopy with post-acquisition super resolution.

Studying large subjects by cryo-EM comes with a range of challenges, for both acquisition and processing. Achieving high resolution results requires higher magnifications which limit field of view, or selection of acquisition time parameters which dramatically increase storage requirements. Post-acquisition super resolution (PASR) allows data to be acquired with more flexibility while still permitting high resolution reconstructions from data which were previously limited.



Keitaro Yamashita

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The University of Tokyo

## Crystallographic structure refinement using Servalcat

Structure refinement, the final step in crystallography, significantly impacts the accuracy of derived models. While current methods usually utilize structure factor amplitudes, Servalcat, a new development, employs intensity-based refinement. This approach holds the potential to utilize the entire observed dataset.

This presentation will discuss the advantages of the intensity-based refinement and recent improvements of the monomer library, which also has an impact on the accuracy of the model.