DATE: Day 16 Month 05 Year 2017

SUMMARY of
2016 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

Research Title		Structure characterizations of shrimp nodaviruses virus-like particles
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	Present Title	Scientist/Professor (Division Head of Scientific Research Div.)
Research Collaborator (Host PI)		Prof. Atsushi Nakagawa

Summary

Shrimp nodaviruses can affect larvae, post-larvae and early juvenile stages of shrimp and cause white tail disease or white muscle disease, reaching to 100% mortalities, which have the impact on the heavy economic losses. In the past year (2016.4~2017.3) under the International Collaborative Research Program with IPR, we have made several attempts of data collection at the beamline 44XU of SPring-8 to determine the crystal structure of capsid proteins and virus particles of shrimp nodaviruses at high resolution. The determined structures allow us to compare with other viral capsid proteins and to investigate the evolution linages of shrimp nodaviruses among different viral capsid proteins to design the new vaccine related to the capsid structures for the improvement of the immune response. The manuscripts of structures of shrimp nodaviruses are under preparation.

Besides the work of shrimp nodaviruses, we also determined several structures and published a few papers in the past year based on the continuous collaboration and the provided BL44XU beamtime. While we determined the crystal structures of a piscine betanodavirus, grouper nervous necrosis virus (GNNV), we developed a novel *ab inito* phasing method with molecular averaging in real space to contribute to phasing with non-crystallographic symmetry averaging or cross crystal averaging. In the published paper, we also proposed a new criterion to judge the successful and failure cases of *ab inito* phasing. The crystal structure of rice α-amylase/subtilisin inhibitor (RASI) was determined to reveal its bi-functional enzyme-inhibiting activities. Characterization of the dimer interactions at the dimeric interface of the crystal structure of RASI were performed using the quantum theory of atoms in molecules (QTAIM) and natural bonding orbital (NBO) analyses at the density-functional theory (DFT) level. Our calculation of the interaction energy might provide a useful approach to identify and to define the best biological molecular model with the greatest stability for a multimeric protein from possible forms generated from a MR solution. Finally, we appreciate the generous support and strong collaboration of IPR and SPring-8 44XU beamline.

***Deadline: May 19, 2017**
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