DATE: Day 26 Month 07 Year 2016

SUMMARY of
2015 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

Research Title		Crystal structures of glycosyltransferase-1 (*Bc*GT-1) from *Bacillus cereus* for the application of drug development
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Research Collaborator (Host PI)		Prof. Atsushi Nakagawa

Summary

Glycosyltransferases (GTs), distributed widely in various organisms, including bacteria, fungi, plants and animals, play a role in synthesizing biological compounds. The glycosyltransferase from *Bacillus cereus* (*Bc*GT-1) is capable of transferring glucose to the small molecules, such as kaempferol and quercetin. In the past year (2015.4~2016.3) under the International Collaborative Research Program with IPR, we have made several attempts of data collection at the SPring-8 beamline 44XU to determine the crystal structure of *Bc*GT-1. The structural analyses provide insights into the catalytic mechanism and the synthesis of the pure quercetin monoglucoside.

Besides the work of *Bc*GT-1, we also published a few papers in the past year based on the continuous collaboration and the provided BL44XU beamtime, among which several crystal structures were determined. The crystal structures of bacteriohemerythrin and its mutants from *Methylococcus capsulatus* (Bath) were determined to reveal that the key residue Leu114 regulates the substrate tunnel. We solved various crystal structures of a piscine betanodavirus, grouper nervous necrosis virus (GNNV), to understand the mechanisms of capsid assembly and viral infection. The crystal structure of an antigenic outer-membrane protein ST50 from *Salmonella* Typhi was determined, suggesting a potential antigenic loop and an efflux mechanism for future application. These results also shed insights into the structural basis for evolutionary lineage of the family *Nodaviridae*. Recently, we have also developed a novel *ab inito* phasing method with molecular averaging in real space to contribute to phase crystal structures with non-crystallographic symmetry averaging or cross crystal averaging. In this method, we proposed a new criteria to distinguish the successful and failure cases. Finally, we appreciate the generous support and strong collaboration of IPR and SPring-8 44XU beamline.

***Deadline: July 31, 2016**
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