DATE: Day 5 Month 6 Year 2020

SUMMARY of
2019 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

Research Title		Crystal structure of the functional particulate methane monooxygenase from *Methylococcus capsulatus*
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	Present Title	Scientist/Professor (Deputy Director)
Research Collaborator (Host PI)		Prof. Atsushi Nakagawa

Summary

The particulate methane monooxygenase (pMMO), as a membrane protein, from methanotrophic bacteria is capable of mediating the conversion of methane to methanol under ambient temperatures and pressures. Several attempts of crystal examination and data collection with BL44XU in 2019 have been made; however, these crystals only diffracted to ~7 Å resolution, which was not suitable for structure determination to inspect the complete cofactors. The pMMO sample was further set up for crystallization using the lipidic cubic phase method. We have recently observed some new crystals from a few conditions. We will examine these crystal qualities by X-ray diffraction in next available beamtime of BL44XU when international traveling is allowed due to the situation of COVID-19 pandemic.

Besides the work of pMMO, we also published one paper [*Acta Cryst*. (2020) D76, 147-154] in the past project year based on the continuous collaboration and the provided BL44XU beamtime. The molecular averaging method in real space coupled with solvent flattering is powerful in phase determination or phase improvement in protein crystallography. Non-crystallographic symmetry (NCS) averaging with the phase extension for structure determination of icosahedral viruses is a common procedure for phase improvement after initial calculations based on molecular replacement using a density map from a cryo-electron microscope, a similar structural model or initial experimental phases from isomorphous replacement or anomalous dispersion.

In this paper, a new approach to optimize or to refine the electron density directly under NCS constraints is proposed. This method has the same effect as the conventional NCS-averaging method, but does not include the process of Fourier synthesis to generate the electron density from amplitudes and corresponding phases. It gives great merits to solve structures with limited data that are either twinned or incomplete at low resolution. This method was successfully applied to the case of the *T*=1 shell-domain (S-domain) sub-viral particle (SVP) of *Penaeus vannamei* nodavirus (PvNV) with the data affected by twinning, which can benefit and apply to other cases in structural biology with protein crystallography.

***Deadline: May 15, 2020**
***Please submit it to E-mail: tanpakuken-kyoten@office.osaka-u.ac.jp.**
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