DATE: Day 4 Month May Year 2022

SUMMARY of

2021 RESEARCH RESULTS REPORT

For International Collaborative Research with IPR, Osaka University

Research Title		Structural and functional research on the survival-essential
		factors from bacterial pathogens for the development of novel
		antibiotics which induce suicide effect (phase II)
Applicant	Name	Bong-Jin Lee
	Affiliation	Seoul National University
	Present Title	Professor
Research Collaborator (Host PI)		Atsushi Nakagawa

Summary

We prepared the protein crystals and sent it to SPring-8. The beamline staffs of the Institute for Protein Research collected the diffraction data at the wavelength of 1.0 Å and the appropriate distance based on the sample sheet sent with the protein crystal sample. Then, the beamline staffs of the Institute for Protein Research processed each diffraction data with AutoProc and XDS and stored the data to the portable HDD.

For a set being capable of molecular replacement, we tried to solve a structure using a structural template which prepared by AlphaFold2 with Phenix or CCP4i program suites.

Data were processed using XDS. Structural determination was tried using various programs including CCP4, CNS, and Phenix with either manual or automated method.

Experimental Results

VapBC43 complex

- Diffracted successfully to ~2.1 Å.
- Phasing was successful.

PfiAT complex

- Diffracted successfully to ~2.2 Å.
- Phasing was successful

PG0858-0859 +ANP

- Diffracted successfully to ~2.3 Å.
- Phasing was successful

PG0858-0859

- Diffracted successfully to ~3.0 Å.
- Phasing was successful