#### DATE: Day 28 Month April Year 2023

# SUMMARY of 2022 RESEARCH RESULTS REPORT For International Collaborative Research with IPR, Osaka University

le	Structural and functional research on the survival-essential
	factors from bacterial pathogens for the development of novel
	antibiotics which induce suicide effect (phase III)
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Affiliation	Seoul National University
Present Title	Professor
llaborator (Host PI)	Atsushi Nakagawa
	Name Affiliation Present Title

#### 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 was 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 was 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**

### VapBC42 complex

- Diffracted successfully to ~4.2 Å.
- Optimization is ongoing.

### **Phd-Doc complex**

- Diffracted successfully to  ${\sim}3.1$  Å.
- Phasing was successful

### **Phd-Doc complex + DNA**

- Diffracted successfully to  $\sim$ 7 Å.
- Optimization is ongoing.

## YafQ – DinJ + DNA

- Diffracted successfully to  ${\sim}3.1$  Å.
- Phasing was successful

## **HEPN-MNT** complex

- Diffracted successfully to  ${\sim}3.14$  Å.
- Phasing was successful

## HEPN + AMP

- Diffracted successfully to  ${\sim}3.2$  Å.
- Phasing was successful

### YoeB + compound

- Diffracted successfully to  $\sim$ 2.2 Å.
- Phasing was successful

\*Deadline: May 12, 2023

- \*Please submit it to E-mail: tanpakuken-kyoten@office.osaka-u.ac.jp.
- \*Please describe this summary within 1 sheet. Please DON'T add some sheets.
- \*This summary will be published on the web.