DATE: Day 5 Month 6 Year 2020

## SUMMARY of

## 2019 RESEARCH RESULTS REPORT

## For International Collaborative Research with IPR, Osaka University

Research Title		Crystallographic fragment screening and structure determination
		for anticancer target proteins
Applicant	Name	Kim, Hyoun Sook
	Affiliation	National Cancer Center, Korea
	<b>Present Title</b>	Senior researcher/ Principal investigator
Research Collaborator (Host PI)		Prof. Atsushi Nakagawa and Prof. Eiki Yamashita
		(Host PI: Prof. Atsushi Nakagawa)

## **Summary**

Fragment-based drug discovery is a widely used method in the pharmaceutical industry for the targeted therapy that target new drug candidates. Fragment-based drug discovery allows a more effective exploration of chemical space with a higher hit rate compared to the conventional chemical high-throughput screening. We tried to solve three-dimensional structures of Ido1/Tdo2, *L. pneumoniae* SetA, mutant K-Ras, Imp1 and Imp2, and Mtk in complex with their respective inhibitors selected from chemical fragment library screen for development of a novel potential therapeutics. Finally, we could collect and process 66 X-ray data sets.

From these data, we could determine crystal structures and get the several ligand-bound structures. As one of these results, the research manuscripts about structural basis on *L. pneumoniae* SetA and human NIBL1 are in preparation, and the next steps to develop inhibitors against Ido1 and K-Ras are in progress.

<sup>\*</sup>Deadline: May 15, 2020

<sup>\*</sup>Please submit it to E-mail: tanpakuken-kyoten@office.osaka-u.ac.jp.

<sup>\*</sup>Please describe this summary within 1 sheet. Please DON'T add some sheets.

<sup>\*</sup>This summary will be published on the web.