DATE: Day 13 Month 5 Year 2022

SUMMARY of
2021 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
	Present Title	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 indoleamine 2,3-dioxygenases, *L. pneumoniae* GTase, *S. aureus* GTases, and specific mutants of a small GTPase, MINERVA, and kinases, alone or 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 70 X-ray data sets. From these data, we could determine crystal structures and get several ligand-bound structures. As one of these results, the research article about structural studies on Human MINERVA Protein FAM129B has been published. Also, manuscripts about structural basis on *L. pneumoniae* GTase, *S. aureus* GTases, and kinases are in preparation, and also the next steps to further optimize inhibitors against some targets are in progress.

***Deadline: May 13, 2022**
***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.**