

DATE: Day 11 Month 5 Year 2021

SUMMARY of
2020 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		
<p>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 dioxygenases, <i>L. pneumoniae</i> GTase, <i>S. aureus</i> GTases, specific mutants of a small GTPase, FAM129B, 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 84 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 <i>L. pneumoniae</i> GTase, <i>S. aureus</i> GTases, and kinases are in preparation, and also the next steps to further optimize inhibitors against some targets are in progress.</p>		

*Deadline: May 14, 2021

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*Please describe this summary within 1 sheet. Please DON'T add some sheets.

*This summary will be published on the web.