

DATE: Day 13 Month 4 Year 2026

SUMMARY of
FY2025 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, The University of Osaka

Research Title		Phase II Structural Investigation of Anticancer Target Proteins and Their Complexes with Therapeutic Inhibitors
Applicant	Name	Hyoun Sook Kim
	Affiliation	National Cancer Center Korea
	Present Title	Senior Scientist/ Principal Investigator
Research Collaborator (Host PI)		Prof. Atsushi Nakagawa and Prof. Eiki Yamashita (Host PI : Prof Atsushi Nakagawa)
Summary Fragment-based drug discovery (FBDD) is an effective strategy for discovering new therapeutic candidates because it enables efficient exploration of chemical space with a higher hit rate than conventional high-throughput screening. In this study, we determined the three-dimensional structures of KRAS, IDO1, IDO2, and PGGHG in apo and/or inhibitor-bound forms using fragment library screening and crystal soaking approaches. X-ray diffraction data sets were successfully collected and processed for all targets, and electron densities corresponding to bound ligands were identified. For IDO1, diffraction data were obtained at 1.8–3.0 Å; for IDO2, at 2.2–3.0 Å; for KRAS, at 2.0–3.0 Å; and for apo and soaked PGGHG crystals, at 1.5–2.5 Å. We were able to collect and process data sets. From these data sets, we could successfully identify the electron densities of bound inhibitors in targets. These results confirm successful acquisition of ligand-bound complex structure data and support the application of FBDD for structure-based drug discovery.		

***Deadline: May 11, 2026**

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