SUMMARY of
2020 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

<table>
<thead>
<tr>
<th>Research Title</th>
<th>Crystallographic fragment screening and structure determination for anticancer target proteins</th>
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<td>(Host PI: Prof. Atsushi Nakagawa)</td>
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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 dioxygenases, *L. pneumonias* GTase, *S. aureus* 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 *L. pneumonias* 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 14, 2021
*Please submit it to E-mail: tanpakuen-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.