DATE: Day 09 Month 05 Year 2024

SUMMARY of
FY2023 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

Research Title		Three-dimensional structure determination of metallo-hydrolase from *Bacillus* sp., carboxylic acid reductase from *Mycobacterium phlei*, and carboxylesterase from *Anoxybacillus geothermalis* D9
Applicant	**Name**	Prof. Dr. Mohd Shukuri Mohamad Ali
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	Present Title	Professor
Research Collaborator (Host PI)		Prof. Dr. Atsushi Nakagawa

Summary

The biotechnological applications of some enzymes in industrial application have been proven in previous studies, such as in pesticide biodegradation, biosensor development, plastic depolymerization, and wastewater treatment. Therefore, understanding its molecular mechanisms and structural dynamics is crucial for further optimization in industrial applications. Structural analysis via X-ray crystallography provides insights into enzyme mechanisms, substrate interactions, and potential engineering strategies. Overall, these studies emphasize the importance of structural elucidation in advancing enzymology, enabling rational design for industrial and environmental applications. Carboxylic acid reductase (*Mp*CAR), carboxylesterases (EstD9) and metallohydrolase (S3wahi-MH) are the one of the key enzymes studied for current industrial potential. Since there are limited structural information pertaining the mechanism and functions of selected domains, efforts to determine their full structures are needed.. were diffracted at beamline BL44XU. Data collected throughout the fiscal year 2023, has yielded datasets for structure solution via molecular replacement and the use of Alphafold model to generate the initial structures using Phenix platform. The structures obtained allows for better insight to elucidate the enzyme reaction mechanism and the relationship between structural folding and substrate promiscuity.

***Deadline: May 10, 2024**
***Please submit it to E-mail: tanpakuken-kyoten@office.osaka-u.ac.jp.**
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