DATE: Day 09 Month 05 Year 2025

SUMMARY of
FY2024 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

Research Title		A New approach to explore proteins binding interfaces flexibility using biased molecular dynamic and normal mode analysis
Applicant	**Name**	**Thibault Tubiana**
	Affiliation	Institute for Integrative Biology of the Cell (I2BC), CNRS/CEA
	Present Title	CNRS Researcher (PI)
Research Collaborator (Host PI)		**Tiwari Sandhya Premnath**

Summary

During my research visit to the Institute for Protein Research (IPR) from September 21 to October 12, hosted by Dr. Sandhya Tiwari, we collaborated on three projects focusing on viral protein flexibility and interactions using computational modeling.

The first project investigated the HEV MetY domain, where we applied Normal Mode Analysis (NMA) to reveal regions of high flexibility—complementing prior molecular dynamics (MD) simulations—and identified additional segments potentially involved in membrane and RNA interactions. These findings will be included in an upcoming manuscript.

The second project focused on modeling STAT5b interactions with QSOX2, a nuclear membrane protein. Using an AlphaFold-based protocol, I am generating structural models that will later be refined through MD simulations and validated experimentally.

The third project, developed with an eye toward a 2025 ICR application, explored a potential conformational switch in an HEV fatty acid-binding-like domain. Initial MD simulations of open and closed forms were unstable, highlighting the need for model refinement before further study.

I also contributed to the IPR community through a seminar on viral protein-protein interaction modeling and a hands-on session on visualizing protein structures using PyMOL and ChimeraX—well-received and now under consideration for expansion into a full-length workshop.

***Deadline: May 9, 2025**
***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.**