DATE: Day 25 Month 04 Year 2017

SUMMARY of
2016 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

Research Title		Development of a pipeline for the refinement of protein-ligand complexes.
Applicant	**Name**	Dr. K. Sekar
	Affiliation	Indian Institute of Science, Bangalore, INDIA
	Present Title	Professor
Research Collaborator (Host PI)		Dr. Atsushi Nakagawa

Summary

In the current 'Next Generation Sequencing' era, the volume of three-dimensional protein structural data has grown exponentially over a period of time. To be specific, with the current technological advances and computing power, the exponential growth of protein structures and a number of structural genomics initiatives worldwide, there is every reason to expect that the amount of protein structural data will only increase.

In addition, although crystallographic data pertaining to drug-target protein complexes are collected by pharmaceutical industries continually, this X-ray data is not refined completely, thereby not providing useful and valuable information. Further, these data and the three-dimensional atomic coordinates are not deposited in the Protein Data Bank archive (PDB). This causes a lacuna in the drug discovery process while trying to identify and develop drugs for a particular disease. Thus, a single efficient pipeline for the refinement of protein-ligand complexes in one go is the need of the hour. To this end, an automatic pipeline has been created for the refinement of protein-ligand complexes.

***Deadline: May 19, 2017**
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