

Project Title:

Development of computational tools to interpret low-resolution structural data

Name: Florence Tama, Osamu Miyashita, Atsushi Tokuhisa

Laboratory at RIKEN:

**Computational Structural Biology Research Unit, Computational Biophysics Research Team,
RIKEN Advanced Institute for Computational Science**

1. Background and purpose of the project, relationship of the project with other projects

Our research focuses on the development of computational tools to study biological systems, more specifically to help in the 3D structural determination of biological systems from various low-resolution experimental data, such as cryo-EM, XFEL, and SAXS, and to analyze their potential interactions with small molecules in order to design new drugs.

These data consist of a large number of images and the biological molecules to be studied are very large. Therefore, large computational resources are required to process the data efficiently.

2. Specific usage status of the system and calculation method

We have been continuing the analyses of XFEL and cryo-EM data. During FY2014, we performed calculations at other facilities.

3. Result

We developed a new approach for flexible fitting of X-ray structures into low-resolution density map using replica exchange molecular dynamics simulation. This new approach can construct the models with higher quality more consistently.

4. Conclusion

We have used RICC to develop programs. During FY2014, we performed most calculations outside RICC.

5. Schedule and prospect for the future

We would like to continue large-scale calculations on RICC. We will apply General Use category a large-scale calculations if the allocated CPU time is not sufficient.

6. If no job was executed, specify the reason.

During FY2014, we were temporarily granted an access to an HPC system in another facility and have

performed most calculation outside RICC.