

## Data processing at pre-data collection with GUI software of Process\_Auto at BL6C

Kiwako SAKABE<sup>1</sup>, Noriyoshi SAKABE<sup>1</sup> and Kyoyu SASAKI<sup>2</sup>

<sup>1</sup>Foundation for Advancement of International Sciences, SBSP House, KEK-PF, Tsukuba, Ibaraki 305-0801, Japan. <sup>2</sup>Graduate School of Environmental Studies, Nagoya Univ., Furo-cho, Chikusa, Nagoya 464-8601, Japan

### Introduction

Galaxy is quite different from other protein data collection system because the detector IP is placed on a fully cylindrical cassette with a small rectangle hole to penetrate primary x-ray beams along the circumference of the cylinder every 10 degrees. So, users have to decide the area size of one frame before starting the data collection. Namely when we select 1.0Å x-ray beam, the maximum resolution of the circumference and the cylinder axis directions are about 0.7 and 2.0Å resolutions, respectively. When we collect very high resolution data, ex. more than 1.3Å resolution, checking the completeness before starting data collection is important, because resolution of cylinder axis direction is limited. Furthermore in time-resolved protein crystallography, we have to record one set of data as fast as possible in minimum number of frames. Thus Weissenberg mode must be selected. This means that the crystal rotation axis must be alignment before data collection. To choose the small frame size to minimize the number of cassettes for recording a full data set is very effective to fast data collection and to reduce disc space.

We have prepared a GUI software of Process-Auto for data processing at pre-data collection.

### Experimental and result

#### GUI software

GUI software was written about minimum modules and input data file from Process-Auto (CUI) by Mr. Yasumasa Nishino [1]. This software named "kaiseki" contains essential modules from the orientation matrix as well as obtaining the cell dimensions to the structure factor calculations; list\_frame, pks, fftindex, index, reduce, remerge, simul, predic, refosc, integ, merge, scale, laue and average. Figure 1 and 2 show the first and second windows of the GUI software.

#### Material and method

The experiment was carried out with collaboration of member of SBSP and data collection of more than 30 kinds of protein crystals selected from more than 100 protein crystals were carried out under many conditions, such as, cryo-condition (100K), cooling conditions (250~270K) and room temperature.

#### Procedure of experiment

- 1) Mount a crystal
- 2) Take two or three images at the  $\omega = 0, 90, 45$  by the oscillation width = 1.5~3 degree

- 3) Digitised diffraction data were stored in the data server in SBSP House.
- 4) Determine the crystallographic parameters and orientation matrix using above data set with COMPAQ beside the BL6C.
- 5) At first, determine the area size of detector from the maximum resolution and secondary, data collection conditions by the simulation of overlapping, and completeness, finally, crystal quality using module integ or average.
- 6) If the result is not sufficient to user's demand, user must select new crystal or to change the orientation of crystal using goniometer arc that can be moved by  $\pm 20$ deg.

ANALYSIS	
File View Tool	Help
Please select	
Experiment Setup	
Manual	
Image display	
Indexing	
Intensity measurement	
Merging and Computation of structure factors	
Exit	

Figure 1. the first window of the GUI software

Experiment setup
Edit resource.dat file
Frame information : list_frame
Help for list_frame
Exit

Figure 2. The second windows of the GUI software

### Acknowledgement

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### References

- [1] Y. Nishino(2001) Structural Biology (Japanese) vol. 7 No. 2 52-53.