# Comparison of diffraction data of trypsin crystal between BL24XU and R-AXIS IV in house.

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Recent successes in the rational design of HIV-1 protease inhibitors have validated the important role of rational design in the drug discovery process. Knowledge of the three-dimensional structure of that protease, particularly with bound ligands, was critical for the rapid progress in the design of inhibitors.

In the recent year, we have studied the use of trypsin as a model for the structure-based design of other serin protease inhibitors. This procedure provided important structural information when the crystallographic analysis of actual target-ligand complex was unavailable. The low molecular packing density form of trypsin crystal (L-form trypsin crystal) was selected in the study, because its active site was exposed to solvent channel and its inhibitor molecule could be easily removed and introduced by the soaking technique.

In order to understand the performance of new beamline BL24XU A hatch equipped with the Rigaku R-AXIS IV detector system, we initially collected diffraction data of L-form trypsin crystal, and compared between the data set of BL24XU A hatch and our R-AXIS IV(Rigaku)

Benzamidine-inhibited trypsin was crystallized according to an ordinary method. Both diffraction data were collected at 100K using the crystal approximately dimensions of 0.1X0.12 X 0.15 mm with the oscillation range of 2degrees.

Data collection using BL24XU A hatch was performed with a wavelength of 0.834 Å and the exposure time were 4 minutes per 2degrees oscillation. Significant reflections were observed up to 1.5Å. The data were processed and scaled by using the program PROCESS (Rigaku). The number of independent reflections were 35424. The completeness of data at 1.5 Å resolution was 80.3% and the merging R-factor was 0.0502.

On the other hand, data collection using R-AXIS IV (Rigaku) in our laboratory was performed with a wavelength of 1.5418Å and the exposure time were 20minutes per 2degree oscillation. Significant reflections were observed up to 1.8Å. Also the data were processed and scaled by using the program PROCESS. The number of independent reflections were 24533. The completeness of data at 1.8 Å resolution was 79.9% and the merging R-factor was 0.0882.

Although it was preliminary study, we can presume good performance of this beamline in consequence of this result.
It's expected that these high resolution and quality of data are very useful and strong tool for more precise drug design.