Crystallgraphic analysis of proteins related to drug-design I

Shintaro Misaki* 4241, Takashi Kawasuji 4402
Shionogi & Co., LTD.

Protein crystals of integrase and proteinase were used for diffraction experiment. Experimental details and results are as followed;

1. Crystals of integrase.

Diffraction Experiment ;

The size of crystal used for diffraction experiment : 0.1 – 0.2 mm.

Wave length : 0.885 Å

Camera distance : 230 mm

Collimator size : 0.1 mm

Exposure time : 6 mins

Oscillation range : 2.2 deg.

Experimental result ;

Due to the bad mosaicity, collected data set was not be able to processed.

2. Crystals of proteinase

Diffraction Experiment ;

The size of crystal used for diffraction experiment : 0.1x0.1x0.03 mm.

Wave length : 0.885 Å

Camera distance : 230 mm

Collimator size : 0.1 mm

Exposure time : 8 mins

Oscillation range : 2.2 deg.

Experimental result ;

Data set was processed with using DENZO.

Cell constants (Å) : a=32.522, b=52.756, c=67.747

Mosaicity : 0.524

Space Group : P212121 (Z=4)

Data Completeness :

Lower Limit	Upper limit	% of I/Sigma=0	% of reflections total
40.00	3.45	1.1	93.4
3.45	2.74	0.9	97.8
2.74	2.39	1.4	98.7
2.39	2.17	1.9	99.1
2.17	2.02	2.5	99.2
2.02	1.90	3.2	98.8
1.90	1.80	5.9	98.3
1.80	1.72	5.9	98.1
1.72	1.66	8.2	96.8
1.66	1.60	10.2	97.1
All hkl		4.1	97.7

Summary of reflections intensities :

Shell(Å)		I	error	R-fac(lin)	R-fac(squ)
40.00	3.45	1553.2	70.8	0.043	0.051
3.45	2.74	655.4	35.9	0.060	0.066
2.74	2.39	349.7	26.5	0.089	0.107
2.39	2.17	252.6	24.3	0.121	0.153
2.17	2.02	201.2	24.4	0.157	0.202
2.02	1.90	141.8	23.0	0.230	0.325
1.90	1.80	92.5	18.4	0.333	0.534
1.80	1.72	69.8	19.5	0.485	0.769
1.72	1.66	49.3	19.1	0.602	0.990
1.66	1.60	39.7	18.2	0.685	0.000
Allreflections		348.7	28.3	0.100	0.080

According to above results, up to 1.7 Å data was used for structure determination. Structure was solved with using molecular replacement method of software package X-PLOR. Refinement is now under going. Present R value is 25.1 %.