# Biomacromolecules (Crystal)

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## 1. Overview

The development of the "user friendly software system" to solve the protein structure by the multiple isomorphous replacement method with optimized ano-malous scattering (MIR-OAS), the major project of C-1 SG, is completed under environment of windows NT by Shimane University group. Now the improvement and the test of the software to apply so called "routine analysis" are held. The menu view, user interface and the output of the symmetrical minimum function to determine heavy atom positions are shown in Fig's. 1, 2 and 3. The other project is to assist the utility check and refinement of the BL41XU hardware system. Since the beamline was opened for users from September 1997, two students, Mr. Hirokazu Ishaida and Masatake Akita of the Graduate School, Nagoya University were dispatched a total of 5 weeks to help the data collection at BL41XU.

## 2. Data Collection

An example of the data collection carried out at 8th to 9th December 1997 by Nagoya University group is shown.
Sample phospholipase D from Strepto-myces antibioticus (PLD); crystal size: 0.05 x0.05x0.07mm; space group P212121, a=60.7, b=99.8, c=108.3A.
Conditions of the data collection ; wave length 1.00A, crystal to film(IP) distance 560mm, oscillation range and speed 5 deg. and 5deg./s, number of oscillation 5, exposure time 1s/IP, a total number of IP used 19.
Data processing using DENZO ; total reflections 65,947, independent ref-lections 16,604, max. resolution 2.5A, Rmerge=0.010, completeness 0.943. The structure of PLD was solved by the single isomorphous replacement method using a Hg derivative. The electron density map calculated at 6A resolution clearly showed the molecular boundary of PLD. The molecular size of PLD is roughly 60x45x40A.

## 3. Preparation of Isomorphous Xenon Derivatives

A simple method for the preparation of isomorphous derivatives is Xe binding to crystallized proteins[1]. Dr. Atsuo Suzuki of Nagoya University tested his prepa-ration system, as shown in Fig. 4, to bind Xe into a crystal of alpha-amylase, though the data collection was not successful because of crystal deterio-ration. The test is still continuing by Dr. Suzuki at Nagoya University.

## References

[1] M. Schultz, T. Prange and R Fourme; J. Appl. Cryst. 27, 950-960 (1994).

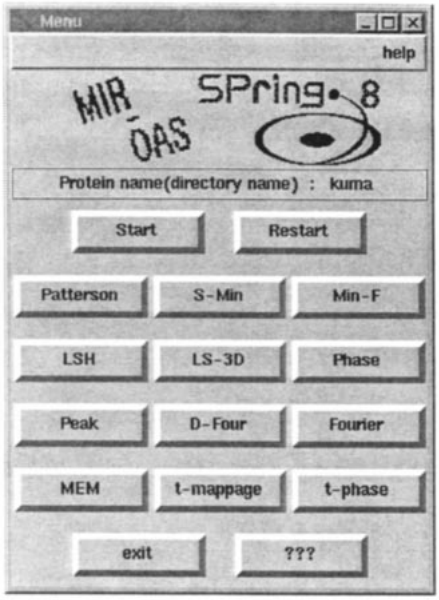


Fig.1.Menu view of the user friendly sofware for the routine analysis with the optimized anomalous scattering (RA-OAS system).

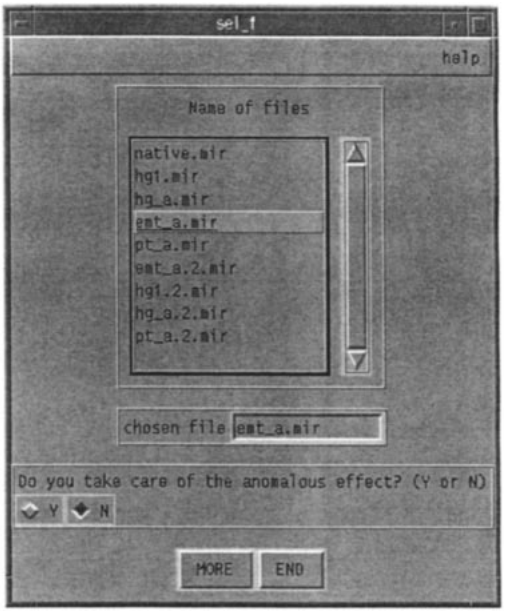


Fig.2.RA-OAS user interface. The sel-f is used to pick up the X-ray data file.

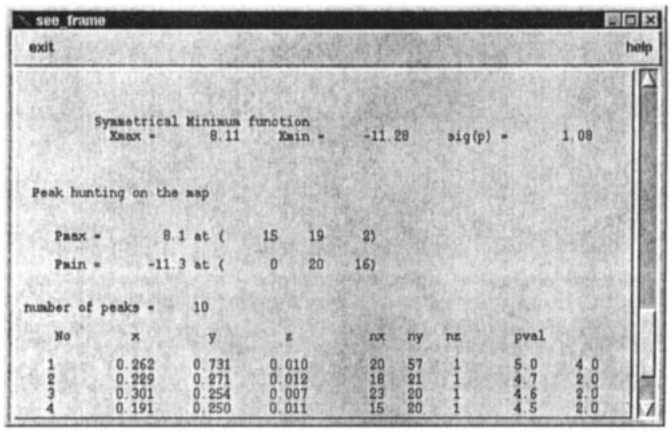


Fig.3.Output list of S-Min (symmetrical minimum function) in RA-OAS system.

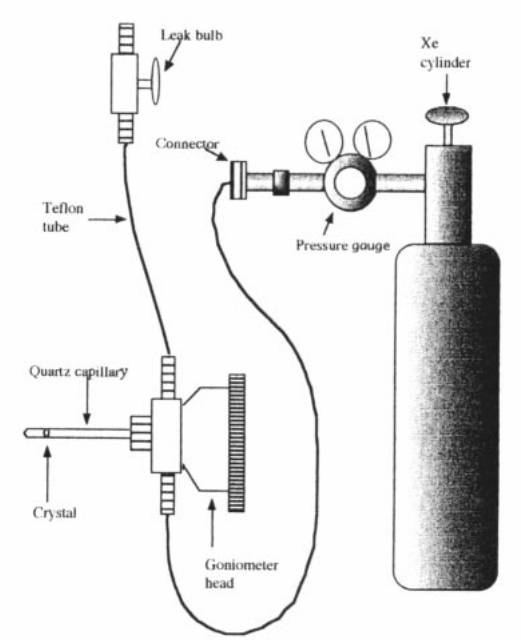


Fig.4.Scematic drawing of the Xe introductory system into a protein crystal.