

Biomacromolecules(Crystal)

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1. Overview

The representative of C-1 SG was changed to Prof. Takashi Yamane of Nagoya University from Prof. Nobuo Tanaka of Tokyo Institute of Technology since June 1996. One member was retired from C-1 SG but three joined newly in this year.

The major project of C-1 SG is the development and improvement of so called "user friendly software" for protein structure analysis. Dr. Kensaku Hamada and Mr. Tohru Atsuta of Shimane University, Prof. N. Tanaka and Dr. Nobuo Kamiya of RIKEN SPring-8 project team are mainly in charge of the development of the software system. This system will be combined with the routine analysis system with optimized anomalous scattering which has been developed by Dr. Nobuo Kamiya.

The activity of C-1 SG was as follows.

2. Joint meeting with C-2 and C-3 S G's

Joint meeting together with C-2 and C-3 SG's arranged by Dr. N. Kamiya were held at CAST during July 19-20 in order to have a frank and lively discussion between users and the SPring-8 project team. Thirteen members of C-1 SG were joined. Prof. T. Yamane gave some comments from the standpoint of the MIR routine analysis. Dr. K. Hamada had a brief lecture on the present status of the user friendly software for routine analysis, and Mr. T. Atsuta demonstrated how the system worked. The flow chart to check the positions of heavy atoms in isomorphous derivative is given in Fig.1. Participants discussed seriously the selection of OS and the development of GUI. We intend to continue the development of this system.

Participants also understand how important having an original software system is though there are many useful systems for protein crystallography. Both C-1 and C-2 SG's supported the application of the beamline for dynamical analysis of protein structure by the C-3 SG.

3. SPring-8 Symposium

Prof. T. Yamane and the former representative Prof. N. Tanaka joined the Spring-8 symposium on 28 Oct. at CAST arranged by the SPring-8 User Society and JASRI. Prof. T. Yamane introduced some research proposals of C-1 SG using the BL41XU, and also commented on some special problems for protein structure research to operate at SPring-8.

4. Research proposals

Each member of C-1 SG is ready to start his research if beamlines are available at SPring-8, and then applied two or three research proposals using the BL41XU for the starting machine time from October 1997. For example, Prof. T. Yamane applied for 1) structure-function analysis of amylases from *Bacillus* origin and 2) structure-function analysis of adenylate kinase from *Bacillus* origin complexed with substrate analogues. Dr. N. Kamiya also made an application for the set up and evaluation of the routine analysis system. The representatives of C-1, C-2 and C-3 SG's will work together with Dr. N. Kamiya to set up the system and to operate it actually for the X-ray data collection of biomacromolecules.

References

[1] T. Atsuta, K. Hamada, N. Tanaka, H. Moriyama, N. Kamiya and T. Ueki, *Nihon Kesshou-Gakkai Nenkai Kouen Youshi-shu*, p. 97 (1996).

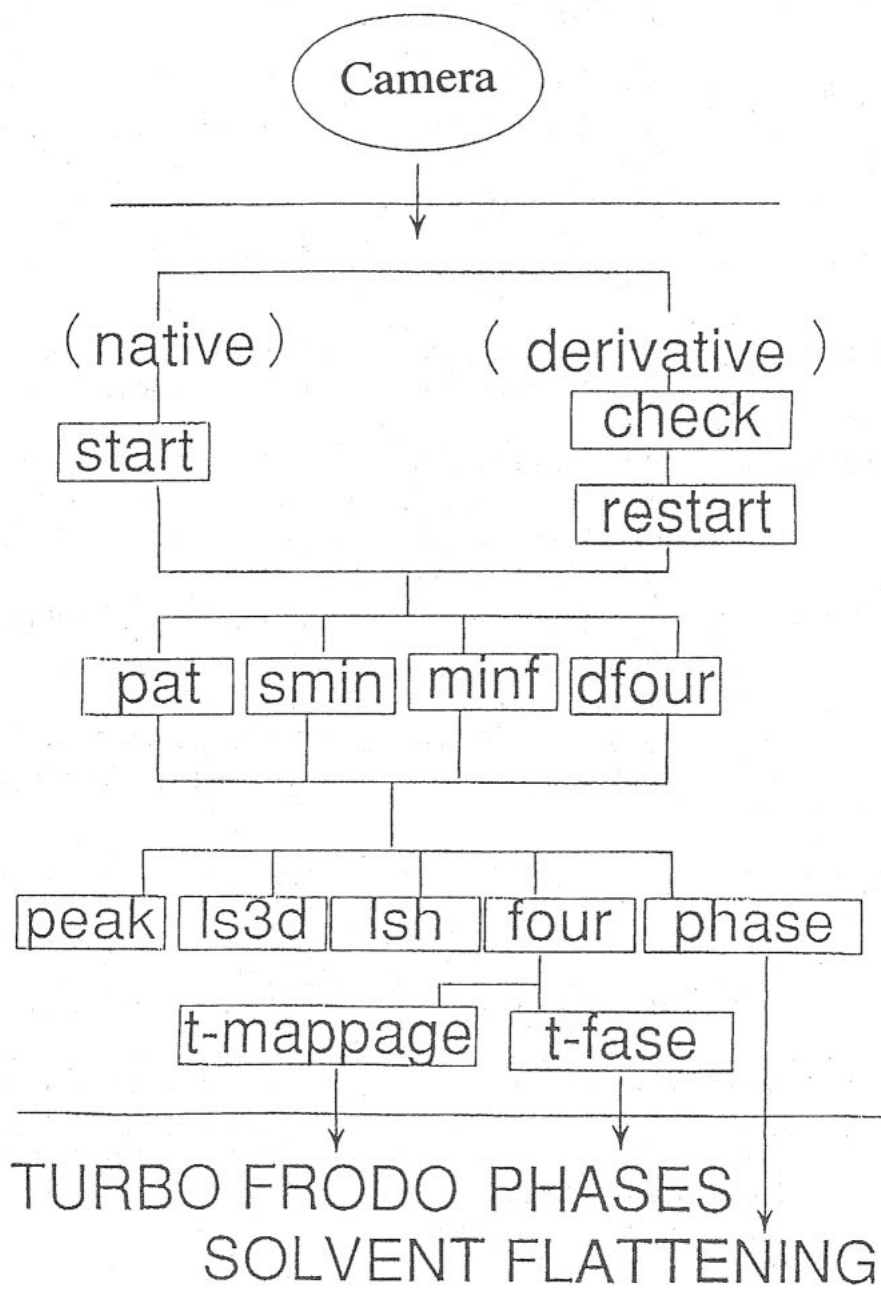


Fig. 1. Flow chart of user friendly software for the routine analysis with optimized anomalous scattering. Window system is adapted. Flow of heavy atom check routine is, **start**→**pat**→**smin**→**peak**→**lsh/ls3d**