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Automated Refinement for Protein Crystallography. Min Yao, Yong Zhou, Isao Tanaka, Graduate School of life Science, Hokkaido Univ., Sapporo, 060-0810, Japan.

During refinement process of protein crystal structures, manual intervention is usually required in the multiple rounds including linking and/or extending the fragments of the initial model and fitting ill-matched residues using computer graphics software. Such manual modification is both consuming time and requiring a great deal of expertise in crystallography. For realizing the manual-intervention-free refinement, we have developed a new automatic refinement software package, LAFIRE (http://altair.sci.hokudai.ac.jp/g6/Research/Lafire_English.html). This software was designed to perform the whole process of protein structural refinement automatically with the refinement programs CNS or REFMAC5 from an initial model that can be approximate, fragmentary or even only main chain. By using LAFIRE, a fully or semi-automatic refinement process can be realized within a few hours or days. The overall strategies and methods used in LAFIRE for model completing and fitting will be presented.